

=> fil reg  
FILE 'REGISTRY' ENTERED AT 10:06:16 ON 15 APR 2004  
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STRUCTURE FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6  
DICTIONARY FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

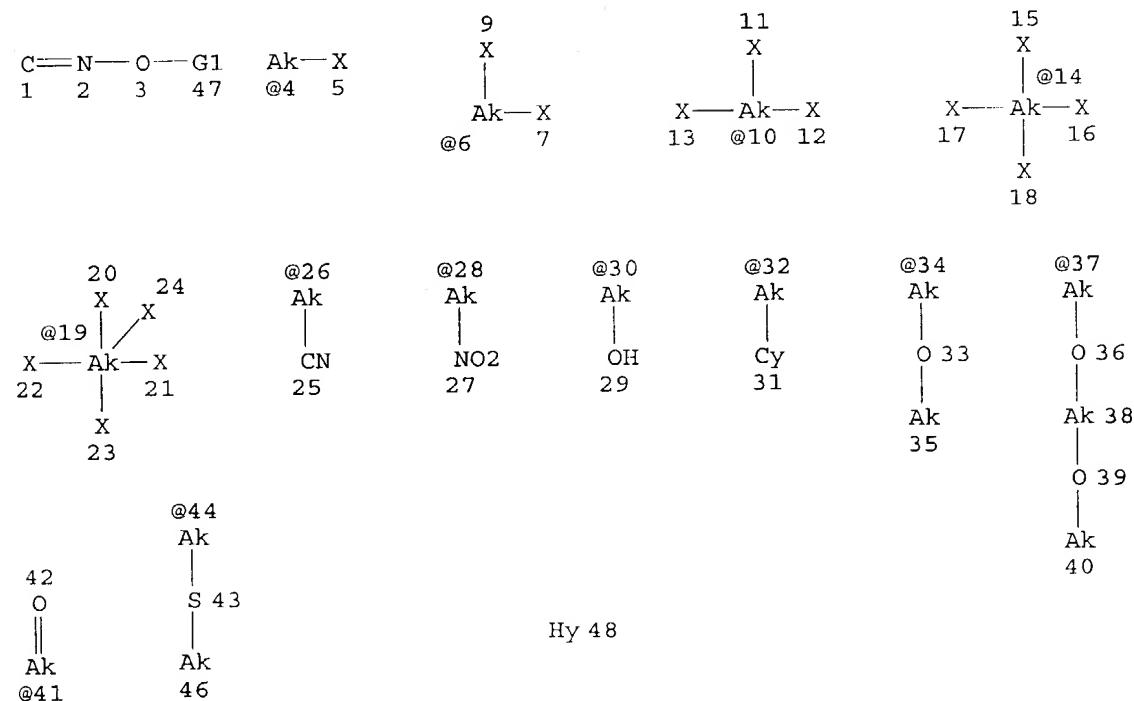
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 147

L25 STR



VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44

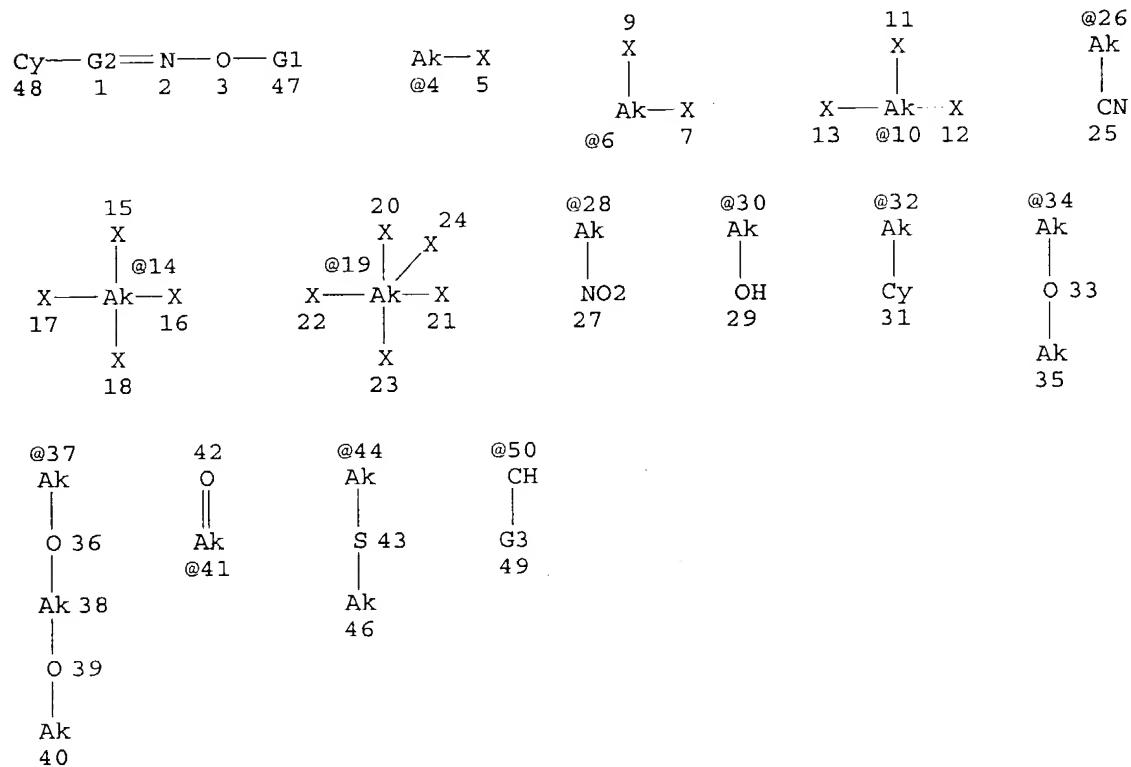
NODE ATTRIBUTES:

NSPEC IS RC AT 1  
CONNECT IS M1 RC AT 1  
CONNECT IS M1 RC AT 19  
CONNECT IS M1 RC AT 48  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE  
L27 46016 SEA FILE=REGISTRY CSS FUL L25  
L36 STR



VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44

VAR G2=CH/50

VAR G3=CN/X/AK/4/6/10/14/19

NODE ATTRIBUTES:

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CONNECT IS M1 RC AT 48

DEFAULT MLEVEL IS ATOM

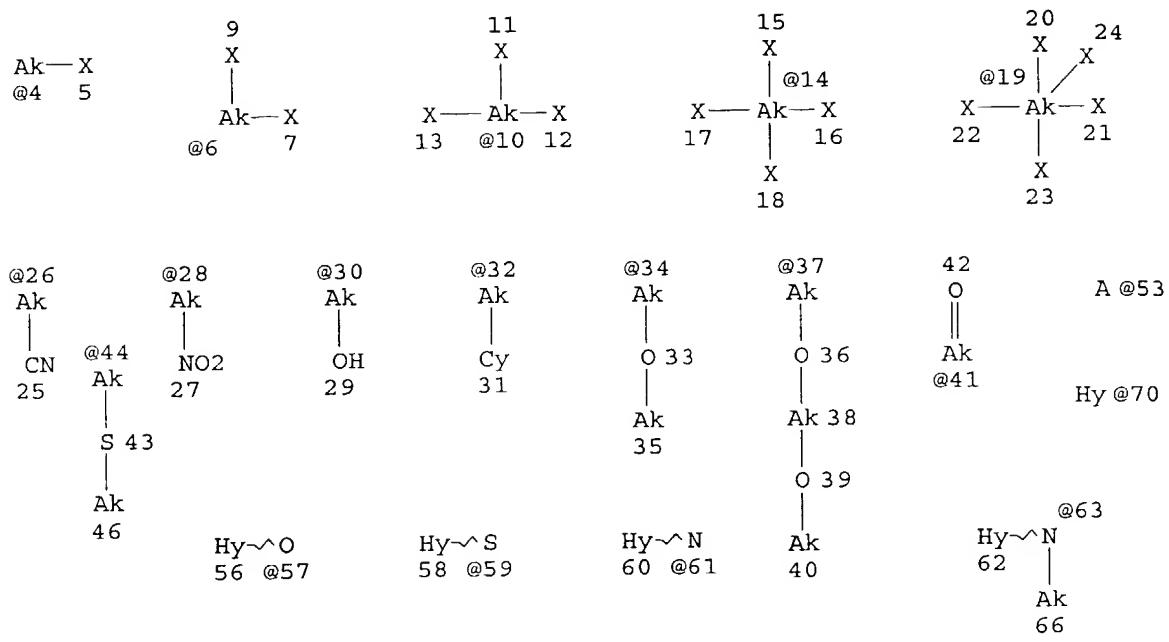
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE  
L38 4398 SEA FILE=REGISTRY SUB=L27 CSS FUL L36  
L45 STR



VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44

VAR G2=70/57/59/61/63/69/55

REP G3=(0-1) AK

REP G4=(0-2) 53

#### NODE ATTRIBUTES:

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NSPEC IS RC AT 1
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 48
CONNECT IS M1 RC AT 53
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CONNECT IS M1 RC AT 55
CONNECT IS M1 RC AT 56
CONNECT IS M1 RC AT 58
CONNECT IS M1 RC AT 60
CONNECT IS M1 RC AT 62
CONNECT IS M1 RC AT 67
CONNECT IS M1 RC AT 70
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
  
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#### GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 65

STEREO ATTRIBUTES: NONE

L47 1307 SEA FILE=REGISTRY SUB=L38 CSS FUL L45

100.0% PROCESSED 4398 ITERATIONS

SEARCH TIME: 00.00.01

1307 ANSWERS

=> d his

(FILE 'HOME' ENTERED AT 08:23:26 ON 15 APR 2004)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 08:23:44 ON 15 APR 2004

L1 1 S WO2000-AU680/AP, PRN  
E WU W/AU  
L2 366 S E3,E28,E29  
E WU WEN/AU  
L3 102 S E3,E115  
E WU WENY/AU  
L4 2 S E6  
E WATSON K/AU  
L5 272 S E3-E18  
E WATSON KEITH /AU  
L6 134 S E3-E14  
E MCCONNELL D/AU  
L7 116 S E3-E8,E13,E14  
E MC CONNELL D/AU  
E JIN B/AU  
L8 307 S E3-E14  
L9 21 S E81  
E KRIPPNER G/AU  
L10 21 S E3-E5  
E BIOTA/PA,CS  
L11 54 S E3-E37  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 08:26:50 ON 15 APR 2004

L12 197 S E1-E197  
L13 23 S L12 NOT OXIME  
L14 5 S L13 AND (C20H22CLN5O2 OR C18H21N3O3 OR C22H29N3O4S OR C21H27N  
L15 18 S L13 NOT L14  
L16 179 S L12 NOT L15  
L17 2 S L16 AND (C9H11NO2 OR C7H7NO)  
L18 177 S L16 NOT L17  
SAV L18 CRANE018/A  
L19 STR  
L20 0 S L19 CSS SAM  
L21 0 S L19 SAM  
STR L19  
L22 0 S L22 CSS SAM  
L23 0 S L22 SAM  
L24 STR L22  
L25 50 S L25 CSS SAM  
L26 46016 S L25 CSS FUL  
SAV TEMP L27 CRANE018A/A  
L28 174 S L12 AND L27  
L29 3 S L18 NOT L28  
L30 2 S L29 NOT C16H21NO2  
L31 176 S L28,L30  
STR L25  
L32 0 S L32 CSS SAM SUB=L27  
STR L32  
L33 0 S L34 CSS SAM SUB=L27  
STR L34  
L36 50 S L36 CSS SAM SUB=L27  
L37 4398 S L36 CSS FUL SUB=L27  
SAV TEMP L38 CRANE018B/A  
L38 STR L36  
STR L39  
L40 1 S L40 CSS SAM SUB=L27  
L41 18 S L40 CSS FUL SUB=L27

L42 = ~~temp~~ 69, 67.4  
X2 (down + right) ~~right~~  
AR  
No  
L31 = ~~leftmost~~ bits  
L31 = ~~leftmost~~ carts

SAV L42 TEMP CRANE018C/A  
 L43 STR L25  
 L44 0 S L43 FUL SUB=L42  
 SAV L44 CRANE018D/A  
 L45 STR L25  
 L46 50 S L45 CSS SAM SUB=L38  
 L47 1307 S L45 CSS FUL SUB=L38  
 SAV L47 TEMP CRANE018E/A  
 L48 1142 S L47 NOT L12

FILE 'HCAPLUS' ENTERED AT 09:21:59 ON 15 APR 2004

L49 2 S L31  
 L50 2 S L49 AND L1-L11  
 L51 391 S L48  
 L52 363 S L51 AND (PD<=19990618 OR PRY<=19990618 OR AY<=19990618)  
 E RHINOVIR/CT  
 E E4+ALL  
 L53 1306 S E7,E6+NT  
 E E5+ALL  
 L54 736 S E6,E5  
 L55 10479 S E5+NT  
 L56 0 S L52 AND L53  
 L57 0 S L52 AND L54  
 L58 0 S L52 AND L55  
 L59 1 S L51 AND L53-L55  
 L60 1 S L51 AND (?RHINOVIR? OR ?PICORNAVIR?)  
 L61 2 S L50,L59,L60  
 L62 41 S L52 AND (?VIRUS? OR ?VIRAL? OR ?VIRUC?)  
 E ANTIVIRAL/CT  
 E E5+ALL  
 L63 43597 S E10,E11,E9+NT  
 L64 10840 S E20  
 E VIRUS INFECTION/CT  
 E VIRA INFECTION/CT  
 E VIRAL INFECTION/CT  
 E E3+ALL  
 L65 10840 S E2  
 L66 42 S L51 AND L63-L65  
 L67 38 S L52 AND L66  
 L68 42 S L62,L67  
 E VIRUS, ANIMAL/CT  
 L69 112431 S E3  
 E E3+ALL  
 E E2+ALL  
 L70 7236 S E5,E3  
 L71 10 S L52 AND L69-L70  
 L72 42 S L68,L71  
 L73 0 S L72 AND (ENTEROVIR? OR COXSA  
 L74 225 S L48 (L) (THU OR BAC OR DMA O:  
 L75 34 S L74 AND L72  
 L76 20 S L75 NOT P/DT  
 L77 14 S L75 NOT L76  
 L78 8 S L72 NOT L75  
 L79 42 S L72 AND L74-L78  
 SEL HIT RN

L61, L62 = only  
 "good" hits for L79  
 which result on structure

of claim 1

References for these  
 in L87

L61 = applicant

FILE 'REGISTRY' ENTERED AT 09:52:05 ON 15  
 L80 75 S E1-E75  
 L81 4 S L80 AND C12H14N6O2  
 L82 3 S L80 AND (C17H14FN3O OR C17H15N3OS OR C18H15N3O2S)

FILE 'HCAPLUS' ENTERED AT 10:03:37 ON 15 APR 2004  
 L83 6 S L81 OR L82

L84 4 S L83 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)  
 L85 2 S L84 AND L53-L55,L63-L65,L69,L70  
 L86 3 S L84 AND (?VIRUS? OR ?VIRAL? OR ?VIRUC? OR ENTEROVIR? OR COXSA  
 L87 4 S L84-L86

FILE 'REGISTRY' ENTERED AT 10:06:16 ON 15 APR 2004

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 10:06:36 ON 15 APR 2004  
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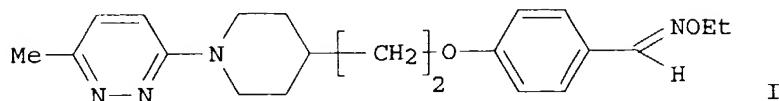
FILE COVERS 1907 - 15 Apr 2004 VOL 140 ISS 16  
 FILE LAST UPDATED: 14 Apr 2004 (20040414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all tot 161 hitstr

L61 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:463807 HCAPLUS  
 DN 139:173249  
 ED Entered STN: 18 Jun 2003  
 TI An Orally Bioavailable Oxime Ether Capsid-Binder with Potent Activity  
 against Human Rhinovirus *MP. 3 amv (wrk R)*  
 AU Watson, Keith G.; Brown, Renee N.; Cameron, Rachel; Chalmers,  
 David K.; Hamilton, Stephanie; Jin, Betty; Krippner, Guy  
 Y.; Lutnick, Angela; McConnell, Darryl B.; Reece, Phillip  
 A.; Ryan, Jane; Stanislawski, Pauline C.; Tucker, Simon P.; Wu,  
 Wen-Yang; Barnard, Dale L.; Sidwell, Robert W.  
 CS Biota Chemistry Laboratory, School of Chemistry, Monash University,  
 Victoria, 3800, Australia  
 SO Journal of Medicinal Chemistry (2003), 46(15), 3181-3184  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 1-5 (Pharmacology)  
 GI

*for Me*



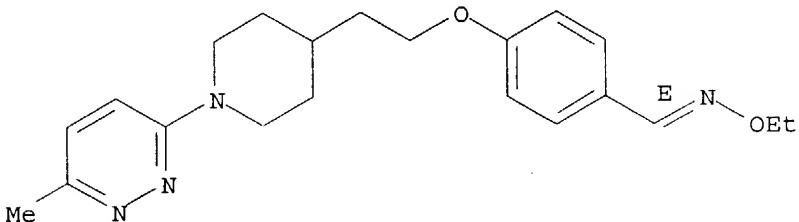
AB A series of capsid-binding compds. was screened against human

**rhinovirus** (HRV) using a CPE based assay. The Et oxime ether (I) was found to have outstanding anti-HRV activity (median IC<sub>50</sub> 4.75 ng/mL), and unlike the equivalent Et ester compound, Pirodavir, it has good oral bioavailability, making it a promising development candidate. I illustrates that an oxime ether group can act as a metabolically stable bioisostere for an ester functionality.

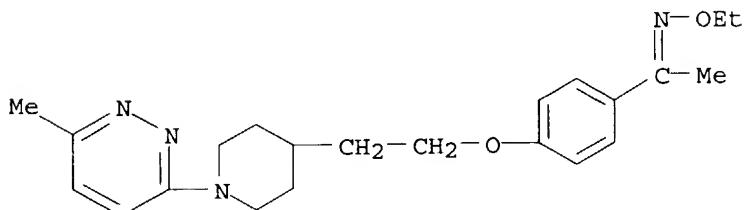
- ST oral bioavailable oxime ether antiviral human **Rhinovirus**
- IT Virion structure  
(capsid; orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT Antiviral agents  
Bioavailability  
Human  
**Human rhinovirus**  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT 577792-16-6P  
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT 124436-59-5P, Pirodavir 124437-42-9P 124437-50-9P 314062-82-3P  
314062-85-6P 314062-87-8P 314062-88-9P  
314062-89-0P 314062-90-3P 314062-91-4P  
314062-93-6P 577792-11-1P 577792-12-2P 577792-13-3P  
577792-14-4P 577792-15-5P 577792-17-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT 120-47-8, Ethyl 4-hydroxybenzoate 141-30-0 622-26-4,  
4-Piperidineethanol 1121-79-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT 124438-51-3P 124438-52-4P 124438-66-0P 124438-73-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- IT 577792-10-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(orally bioavailable oxime ether capsid binder with potent activity against human **Rhinovirus**)
- RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
- (1) Andries, K; Antimicrob Agents Chemother 1992, V36, P100 HCPLUS
  - (2) Andries, K; Antiviral Res 1991, V16, P213 HCPLUS
  - (3) Andries, K; The Search for Antiviral Drugs 1993, P179
  - (4) Anon; WO 0078746 2001 HCPLUS
  - (5) Arruda, E; Antiviral Chemotherapy 1995, P321
  - (6) Bromidge, S; J Med Chem 1997, V40, P4265 HCPLUS
  - (7) Burger, A; Prog Drug Res 1991, V37, P287 HCPLUS
  - (8) Diana, G; Antiviral Chem Chemother 1997, V8, P401 HCPLUS
  - (9) Diana, G; J Comput-Aided Mol Design 1993, V7, P325 HCPLUS
  - (10) Dragovich, P; J Med Chem 1999, V42, P1213 HCPLUS
  - (11) Giranda, V; Acta Crystallogr 1995, VD51, P496
  - (12) Giranda, V; Structure-Based Drug Design 1997, P487
  - (13) Hadfield, A; Proc Natl Acad Sci U S A 1999, V96, P14730 HCPLUS
  - (14) Hayden, F; Abstracts of 40th Interscience Conference on Antimicrobial Agents and Chemotherapy, Abstract 1161 2000

- (15) Hayden, F; Antimicrob Agents Chemother 1992, V36, P727 MEDLINE  
 (16) Hayden, F; Antimicrob Agents Chemother 1995, V39, P290 HCAPLUS  
 (17) Hayden, F; www.viropharma.com/healthcare/clinical.html  
 (18) Karabatsos, G; Tetrahedron 1967, V23, P1079 HCAPLUS  
 (19) Lipinski, C; Annu Rep Med Chem 1986, V21, P283 HCAPLUS  
 (20) Makela, M; J Clin Microbiol 1998, V36, P539 MEDLINE  
 (21) McKinlay, M; Annu Rev Microbiol 1992, V46, P635 HCAPLUS  
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 (23) Patani, G; Chem Rev 1996, V96, P3147 HCAPLUS  
 (24) Sidwell, R; Appl Microbiol 1976, V22, P797  
 (25) Stokbroekx, R; US 4992433 1990 HCAPLUS  
 (26) Tebbe, M; J Med Chem 1997, V40, P3937 HCAPLUS  
 (27) Turner, R; Pediatr Ann 1998, V27, P790 MEDLINE
- IT 577792-16-6P  
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus)
- RN 577792-16-6 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime, [C(E)]- (9CI) (CA INDEX NAME)

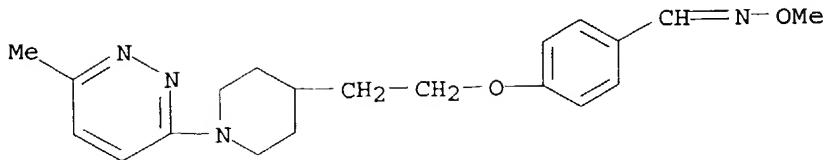
Double bond geometry as shown.



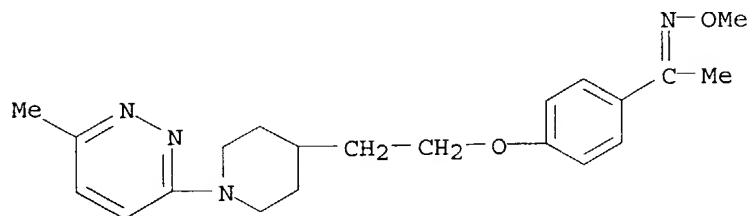
- IT 314062-82-3P 314062-85-6P 314062-87-8P  
 314062-88-9P 314062-89-0P 314062-90-3P  
 314062-91-4P 314062-93-6P 577792-13-3P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus)
- RN 314062-82-3 HCAPLUS  
 CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)



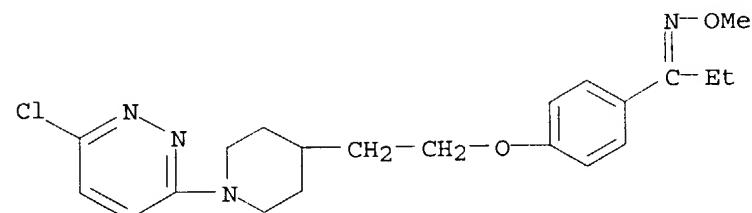
- RN 314062-85-6 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



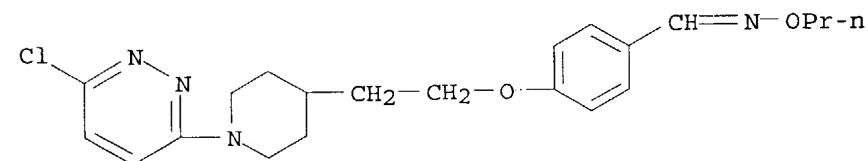
RN 314062-87-8 HCAPLUS  
 CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)



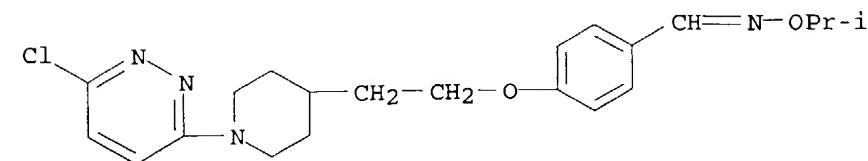
RN 314062-88-9 HCAPLUS  
 CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)



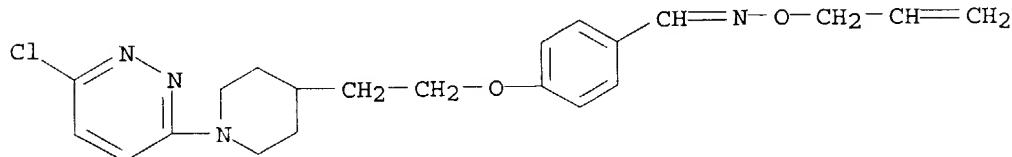
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 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)



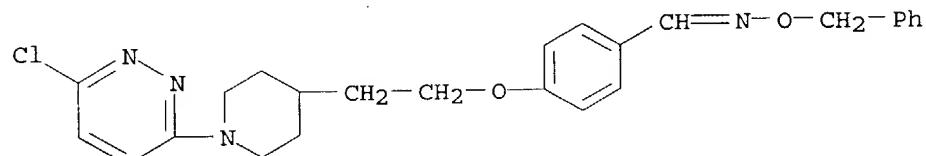
RN 314062-90-3 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(1-methylethyl)oxime (9CI) (CA INDEX NAME)



RN 314062-91-4 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenylloxime (9CI) (CA INDEX NAME)

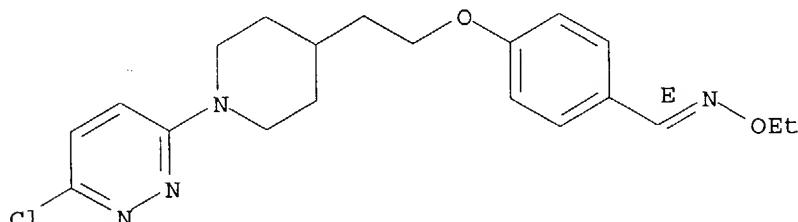


RN 314062-93-6 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(phenylmethyl)oxime (9CI) (CA INDEX NAME)



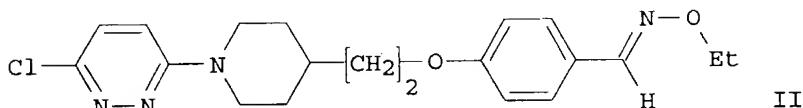
RN 577792-13-3 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L61 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:911241 HCAPLUS  
 DN 134:71606  
 ED Entered STN: 29 Dec 2000  
 TI Preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents  
 IN Wu, Wen-Yang; Watson, Keith; McConnell, Darryl ; Jin, Betty; Krippner, Guy  
 PA Biota Scientific Management Pty. Ltd., Australia  
 SO PCT Int. Appl., 84 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D401-04  
 ICS C07D403-04; C07D261-08; C07D237-10; C07D417-04; A61K031-501; A61K031-42; A61K031-50; A61K031-4453; A61P031-12  
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 10  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000078746	A1	20001228	WO 2000-AU680	20000616
			W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	
EP 1187827	A1	20020320	EP 2000-936548	20000616 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO		
JP 2003502418	T2	20030121	JP 2001-504912	20000616 <--
PRAI AU 1999-1054	A	19990618		
WO 2000-AU680	W	20000616 <--		
OS MARPAT 134:71606				
GI				



AB The title compds. Het-A-Alk-W-Ar-C(X2):NOX1 [I; Het = (un)substituted 5-6 membered monocyclic heterocyclic radical, (un)substituted 9-10 membered bicyclic heterocyclic radical; A = O, S, NH, etc.; Alk = alkylene, a bond; W = O, S, OCH<sub>2</sub>, etc.; Ar = (un)substituted 5-6 membered monocyclic aryl, (un)substituted 9-10 membered bicyclic aryl; X1 = alkyl, alkenyl, alkynyl, etc.; X2 = H, CN, F, etc.], useful in the treatment picornavirus infections in mammals, were prepared Thus, reacting 4-{2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy}benzaldehyde in EtOH with a solution of EtONH<sub>2</sub> in H<sub>2</sub>O afforded 44% O-ethyloxime II. Biol. data (activity against, e.g., HRV-1A, HRV-2, HRV-14, enterovirus 70, Coxsackie A21) for compds. I was given.

ST benzaldehyde oxime heterocyclalkoxy prepn antiviral picornavirus; rhinovirus antiviral benzaldehyde oxime heterocyclalkoxy prepn; enterovirus antiviral benzaldehyde oxime heterocyclalkoxy prepn; coxsackievirus antiviral benzaldehyde oxime heterocyclalkoxy prepn

IT Antiviral agents

Enterovirus

Human coxsackievirus A21

Human rhinovirus 14

Human rhinovirus 2

Picornaviridae

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT Human rhinovirus

(type 1A; preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 314062-80-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 314062-79-8P 314062-81-2P 314062-82-3P

314062-83-4P 314062-84-5P 314062-85-6P  
314062-86-7P 314062-87-8P 314062-88-9P  
314062-89-0P 314062-90-3P 314062-91-4P  
314062-92-5P 314062-93-6P 314062-94-7P  
314062-95-8P 314062-96-9P 314062-97-0P  
314062-98-1P 314063-00-8P 314063-01-9P  
314063-02-0P 314063-04-2P 314063-05-3P  
314063-06-4P 314063-07-5P 314063-08-6P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 314062-99-2 314063-03-1 314063-14-4  
314063-21-3 314063-24-6 314063-29-1  
314063-30-4 314063-31-5 314063-34-8  
314063-49-5 314063-50-8 314063-54-2  
314063-56-4 314063-58-6 314063-62-2  
314063-63-3 314063-65-5 314063-88-2  
314063-92-8 314063-93-9 314063-94-0  
314063-97-3 314064-00-1 314064-02-3  
314064-10-3 314064-11-4 314064-12-5  
314064-35-2 314064-38-5 314064-42-1  
314255-60-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 123-08-0, 4-Hydroxybenzaldehyde 141-30-0 622-26-4, 4-Piperidineethanol  
932-90-1, Benzaldehyde oxime 2508-29-4, 5-Amino-1-pentanol 41731-52-6,  
Ethyl 2-chloro-4-thiazolecarboxylate 54044-79-0, 2-Bromo-5-methyl-1,3,4-thiadiazole 124437-50-9 124438-51-3 124438-73-9 314064-67-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 5198-85-6P 113079-60-0P 314064-59-0P 314064-60-3P 314064-61-4P  
314064-62-5P 314064-63-6P 314064-64-7P 314064-65-8P 314064-66-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Bayer Ag; EP 290906 A 1988 HCPLUS
- (2) Bayer Aktiengesellschaft; US 4472416 A 1984 HCPLUS
- (3) Kumiai Chem Ind Co Ltd; JP 8081314 A 1996
- (4) Malamas; J Med Chem 1996, V39(1), P237 HCPLUS
- (5) Starling; Indian Journal of chemistry 1977, V15(8), P715 HCPLUS
- (6) Strupczewski; J Med Chem 1995, V38(7), P1119 HCPLUS
- (7) Teijin Limited; WO 9001874 1990 HCPLUS
- (8) Teijin Ltd; JP 05320117 A 1993 HCPLUS

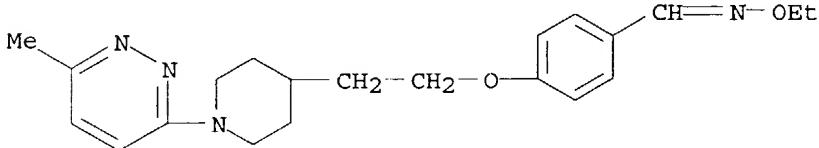
IT 314062-80-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

RN 314062-80-1 HCPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



IT 314062-79-8P 314062-81-2P 314062-82-3P  
314062-83-4P 314062-84-5P 314062-85-6P  
314062-86-7P 314062-87-8P 314062-88-9P  
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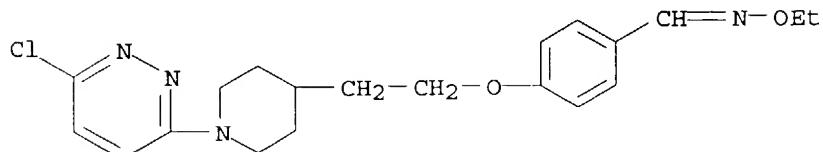
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 BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

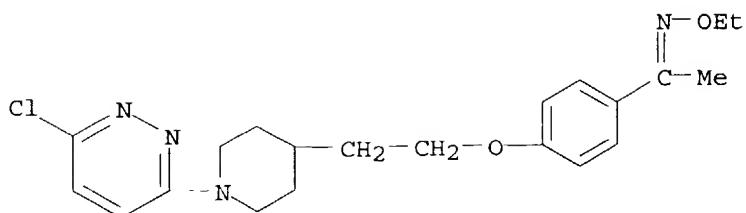
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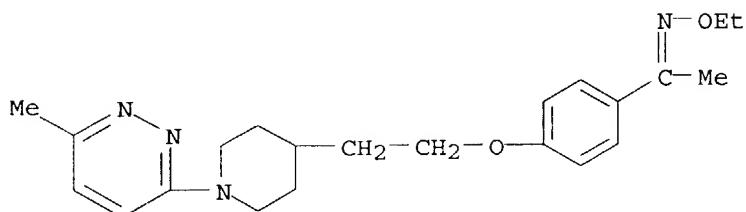


RN 314062-81-2 HCAPLUS

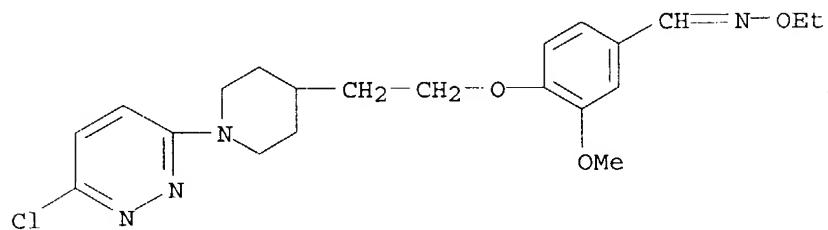
CN Ethanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)



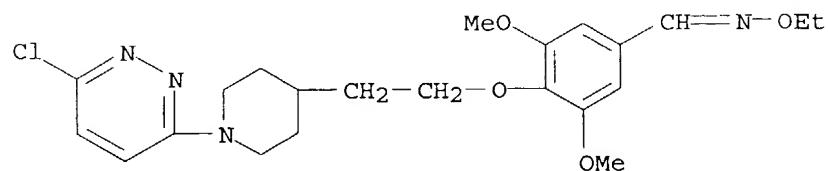
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 CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)



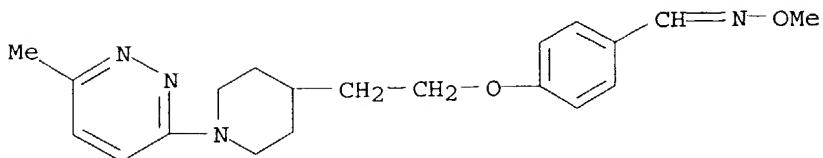
RN 314062-83-4 HCPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methoxy-, O-ethyloxime (9CI) (CA INDEX NAME)



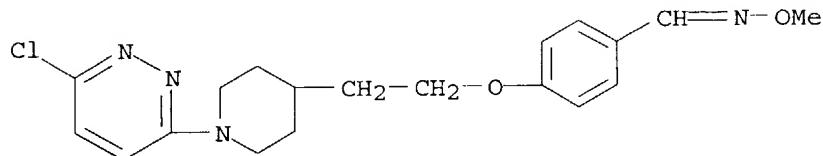
RN 314062-84-5 HCPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-dimethoxy-, O-ethyloxime (9CI) (CA INDEX NAME)



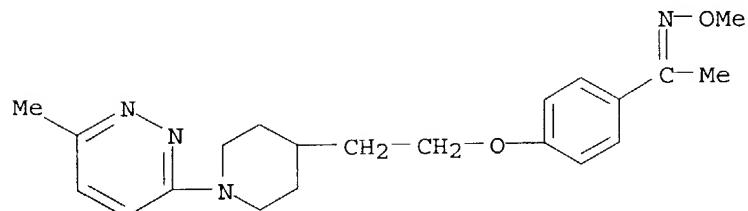
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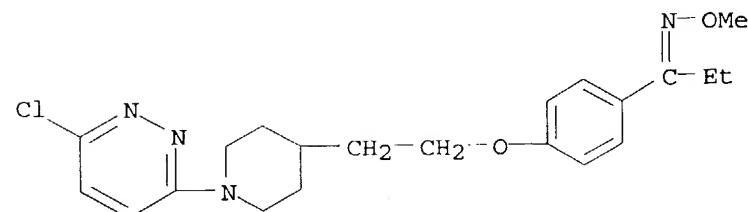
RN 314062-86-7 HCAPLUS  
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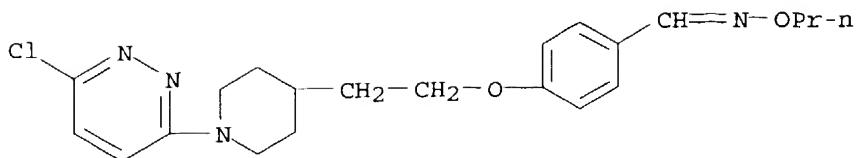
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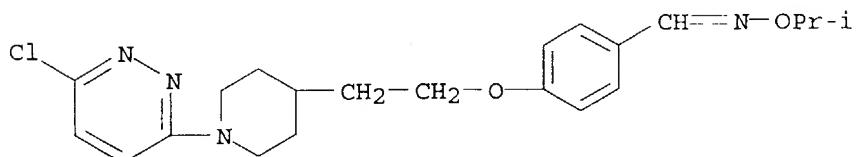
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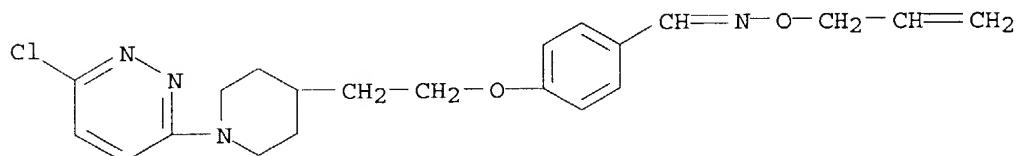
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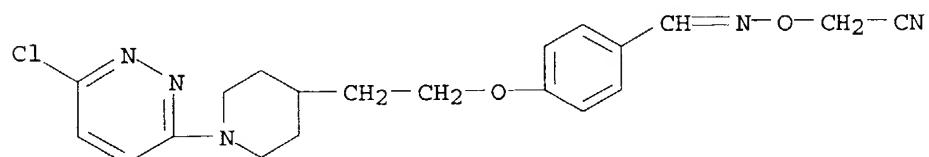
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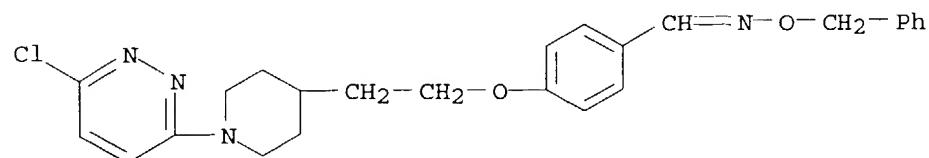
RN 314062-91-4 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyl oxime (9CI) (CA INDEX NAME)



RN 314062-92-5 HCAPLUS  
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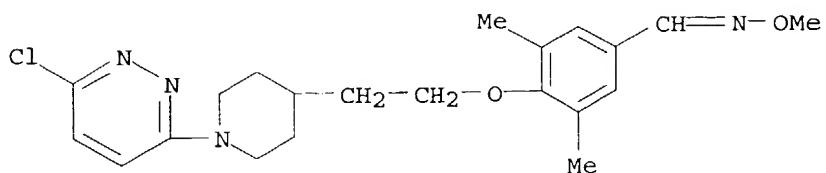


RN 314062-93-6 HCAPLUS  
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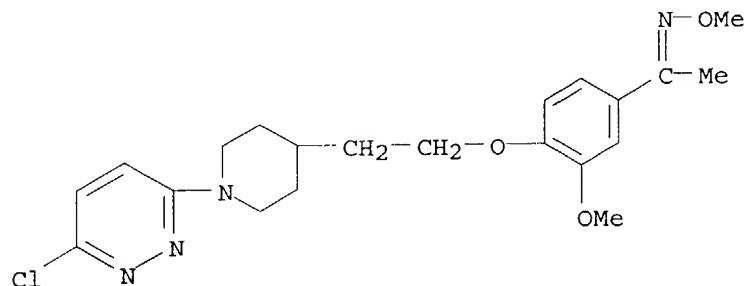
RN 314062-94-7 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-

dimethyl-, O-methyloxime (9CI) (CA INDEX NAME)



RN 314062-95-8 HCPLUS

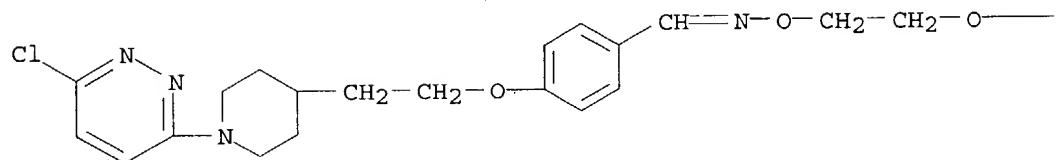
CN Ethanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methoxyphenyl]-, O-methyloxime (9CI) (CA INDEX NAME)



RN 314062-96-9 HCPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-[2-[2-(ethyldioxy)ethoxy]ethyl]oxime (9CI) (CA INDEX NAME)

PAGE 1-A

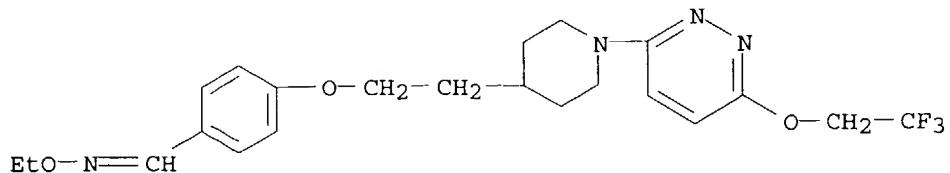


PAGE 1-B

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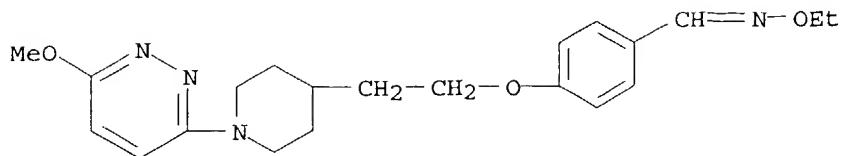
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RN 314062-98-1 HCPLUS

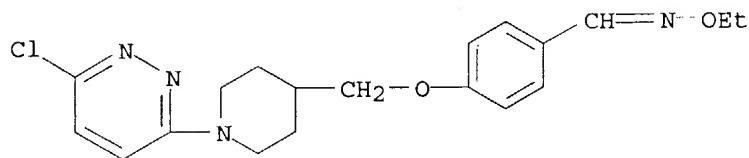
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O-ethyloxime (9CI) (CA INDEX NAME)



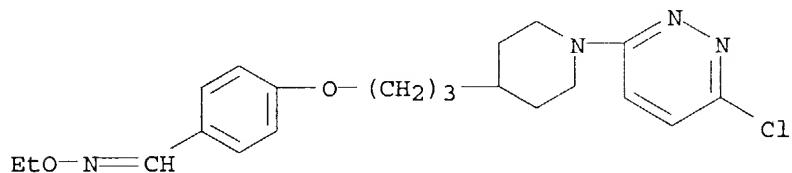
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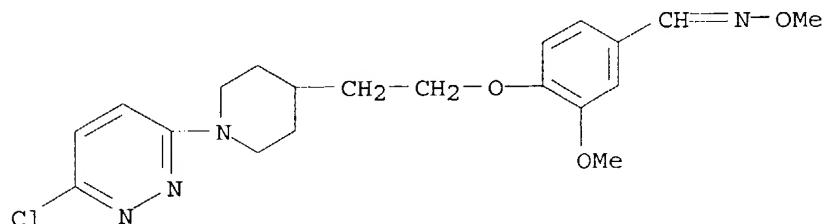
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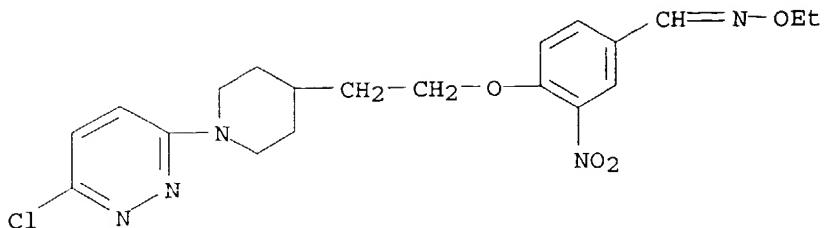
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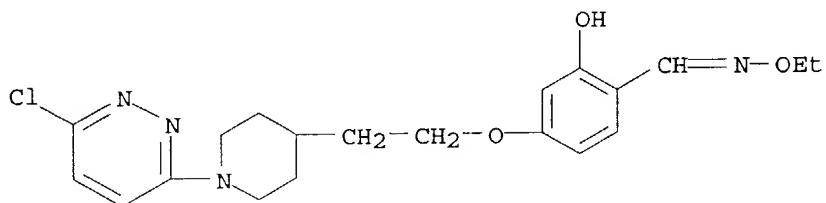
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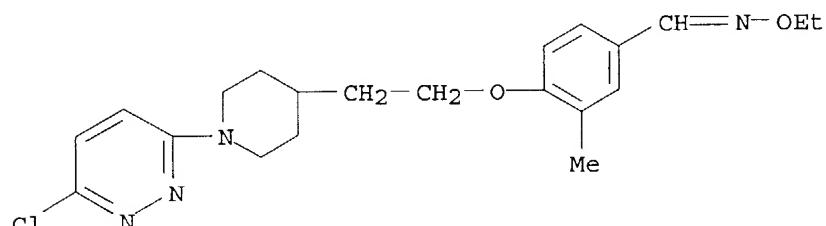
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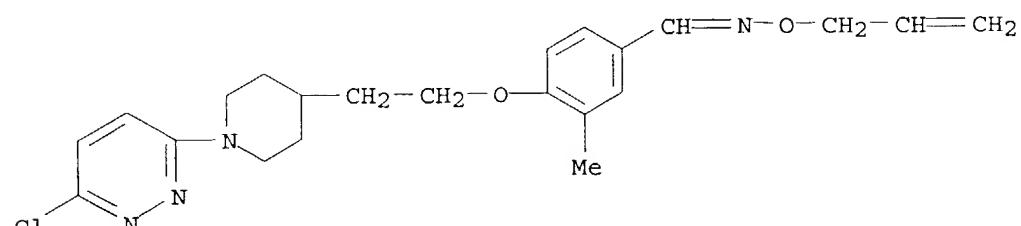
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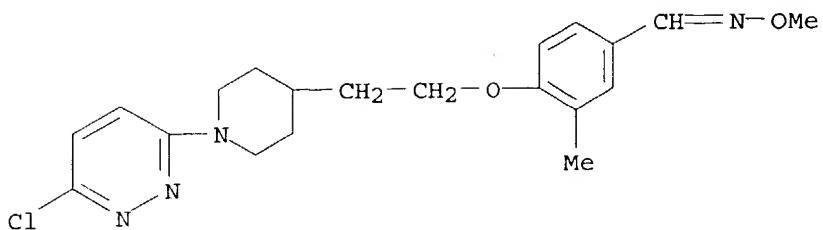
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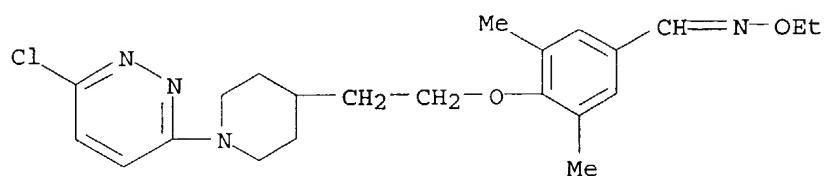


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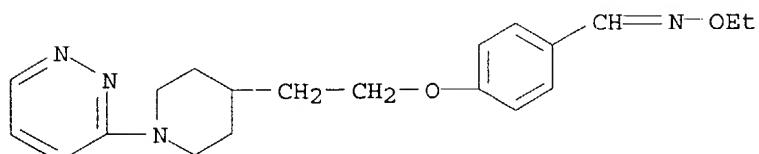
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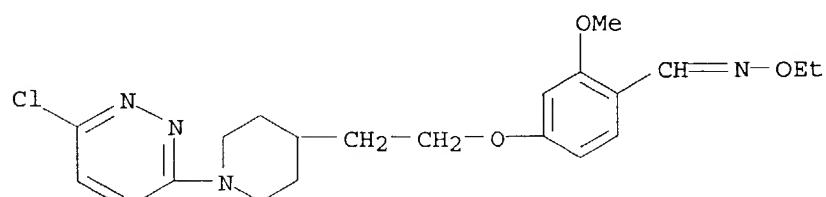
RN 314063-09-7 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)



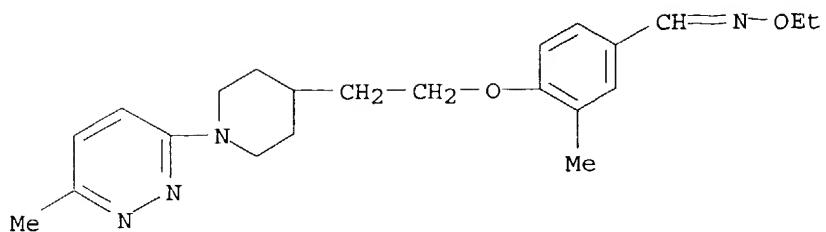
RN 314063-10-0 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314063-11-1 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-2-methoxy-, O-ethyloxime (9CI) (CA INDEX NAME)

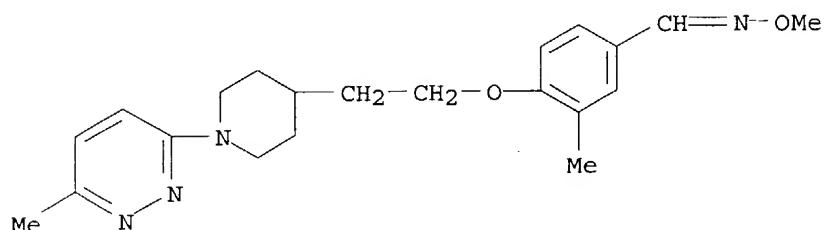


RN 314063-12-2 HCAPLUS  
 CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



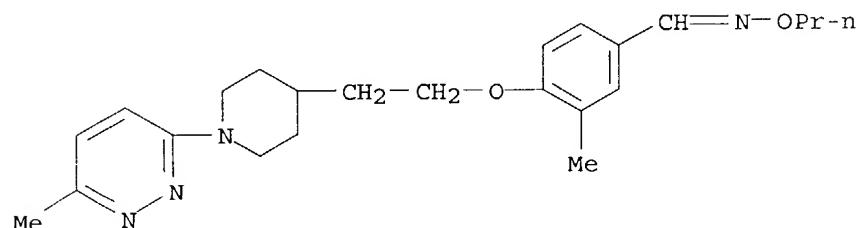
RN 314063-13-3 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



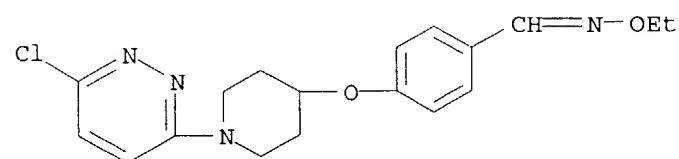
RN 314063-15-5 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)



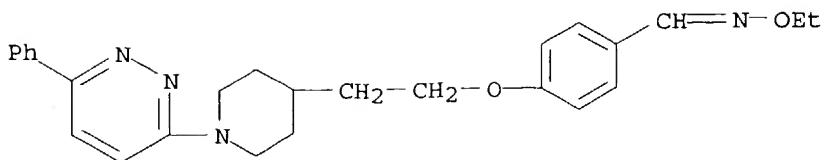
RN 314063-16-6 HCAPLUS

CN Benzaldehyde, 4-[(1-(6-chloro-3-pyridazinyl)-4-piperidinyl)oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314063-17-7 HCAPLUS

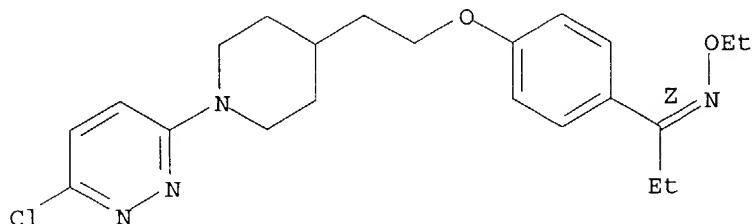
CN Benzaldehyde, 4-[2-[1-(6-phenyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314063-18-8 HCAPLUS

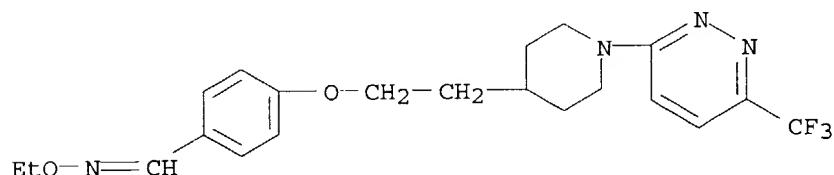
CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime, (1Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



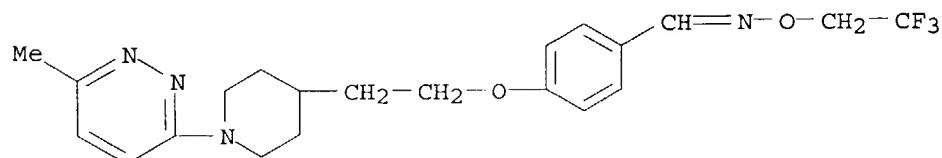
RN 314063-19-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-(trifluoromethyl)-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



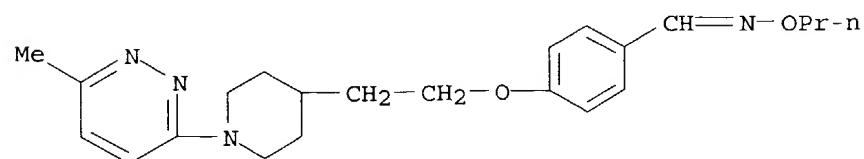
RN 314063-20-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2,2,2-trifluoroethyl)oxime (9CI) (CA INDEX NAME)



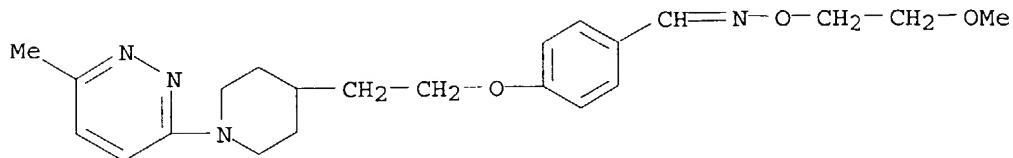
RN 314063-22-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)



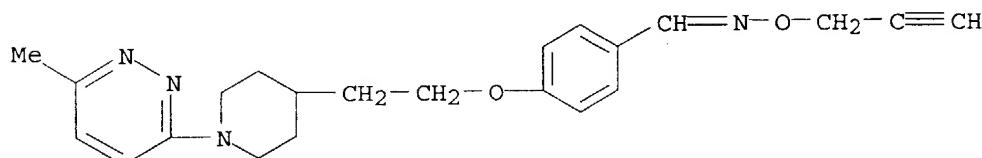
RN 314063-23-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2-methoxyethyl)oxime (9CI) (CA INDEX NAME)



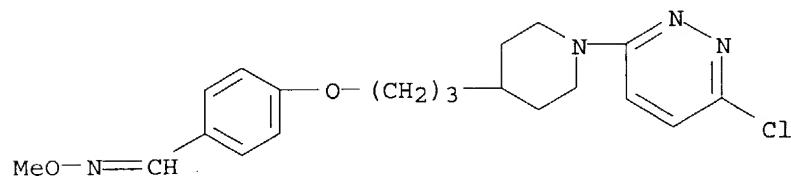
RN 314063-25-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propynylloxime (9CI) (CA INDEX NAME)



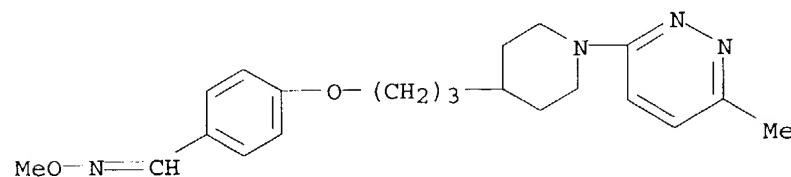
RN 314063-26-8 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



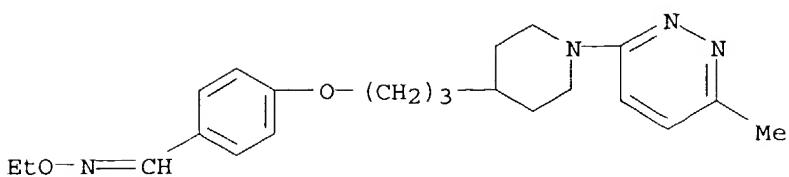
RN 314063-27-9 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



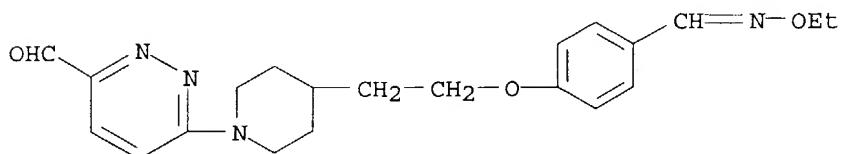
RN 314063-28-0 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



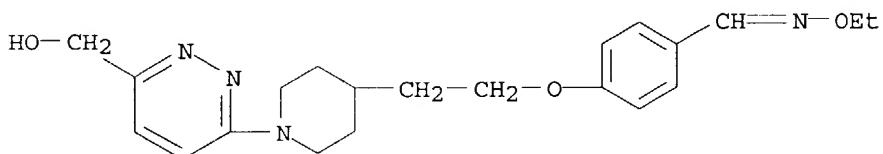
RN 314063-32-6 HCAPLUS

CN 3-Pyridazinecarboxaldehyde, 6-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl] (9CI) (CA INDEX NAME)



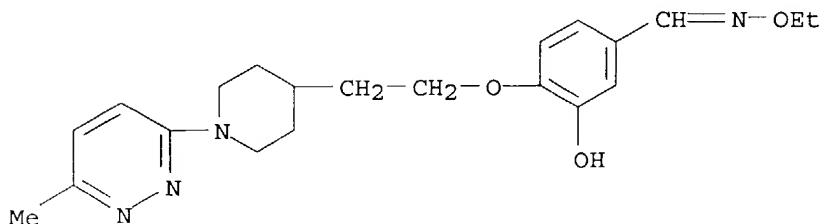
RN 314063-33-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-(hydroxymethyl)-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



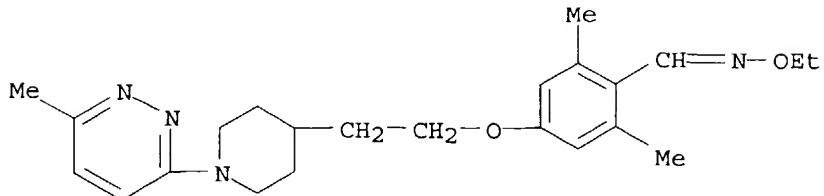
RN 314063-35-9 HCAPLUS

CN Benzaldehyde, 3-hydroxy-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



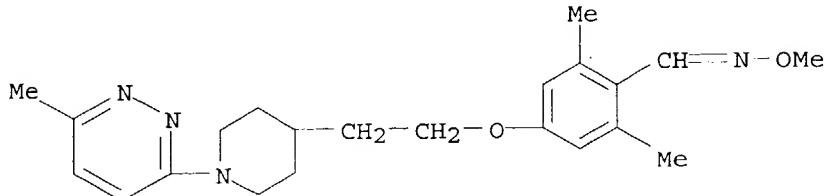
RN 314063-36-0 HCAPLUS

CN Benzaldehyde, 2,6-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



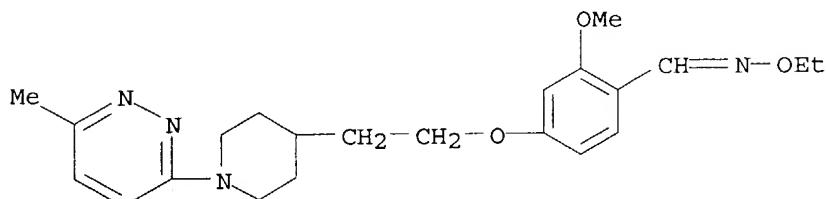
RN 314063-37-1 HCAPLUS

CN Benzaldehyde, 2,6-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



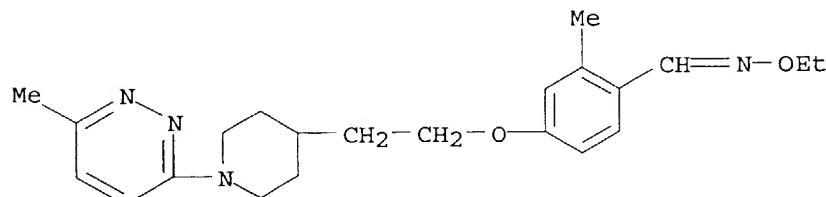
RN 314063-38-2 HCAPLUS

CN Benzaldehyde, 2-methoxy-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



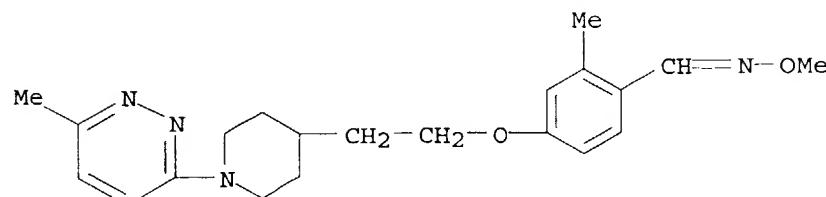
RN 314063-39-3 HCAPLUS

CN Benzaldehyde, 2-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



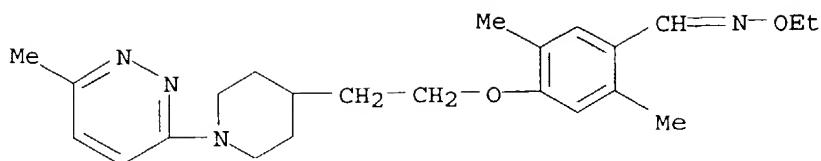
RN 314063-40-6 HCAPLUS

CN Benzaldehyde, 2-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

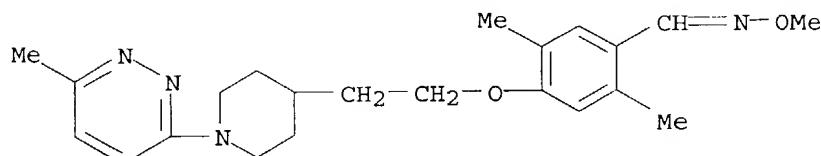


RN 314063-41-7 HCAPLUS

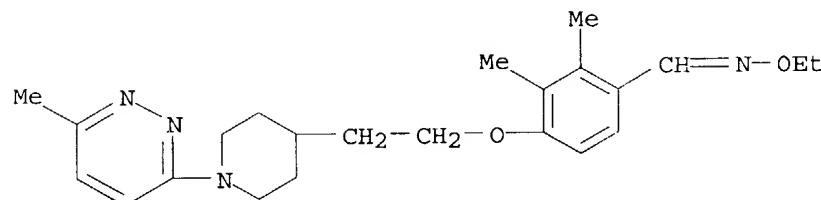
CN Benzaldehyde, 2,5-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



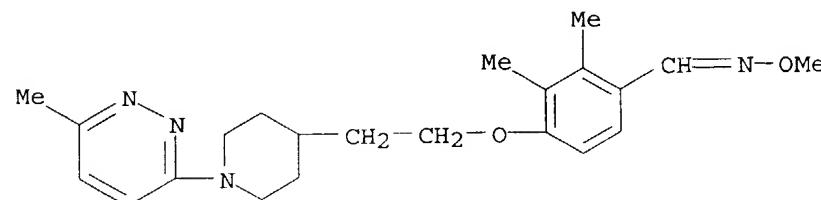
RN 314063-42-8 HCAPLUS  
 CN Benzaldehyde, 2,5-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



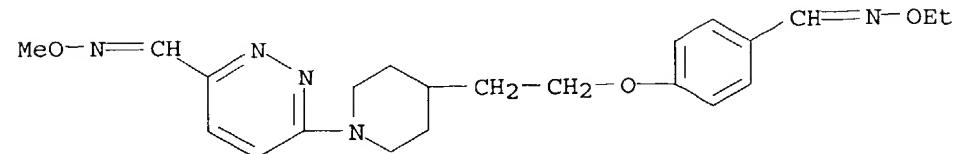
RN 314063-43-9 HCAPLUS  
 CN Benzaldehyde, 2,3-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



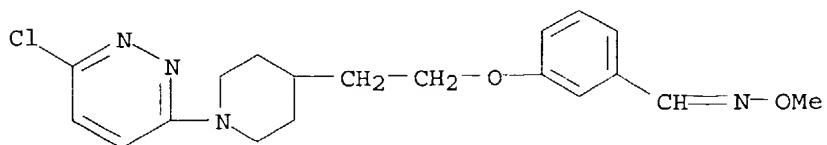
RN 314063-44-0 HCAPLUS  
 CN Benzaldehyde, 2,3-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



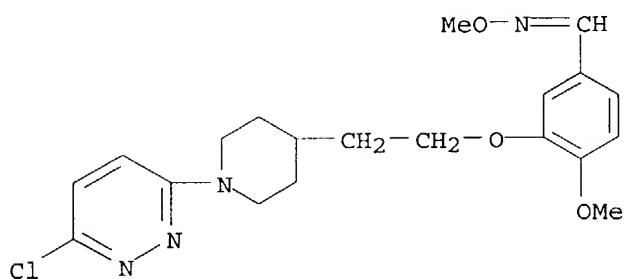
RN 314063-45-1 HCAPLUS  
 CN 3-Pyridazinecarboxaldehyde, 6-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, O-methyloxime (9CI) (CA INDEX NAME)



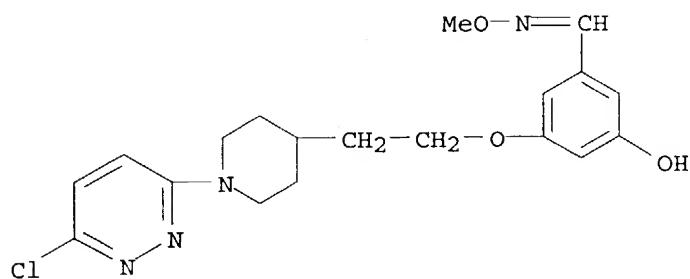
RN 314063-46-2 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



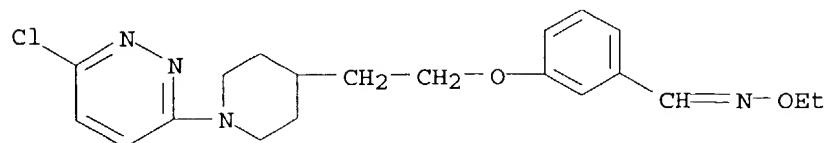
RN 314063-47-3 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-4-methoxy-, O-methyloxime (9CI) (CA INDEX NAME)



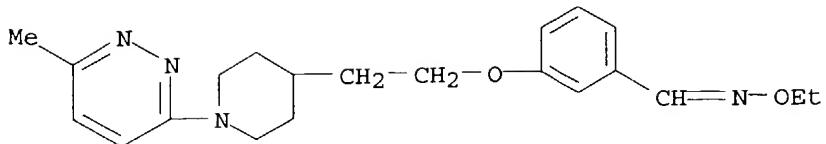
RN 314063-48-4 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-hydroxy-, O-methyloxime (9CI) (CA INDEX NAME)



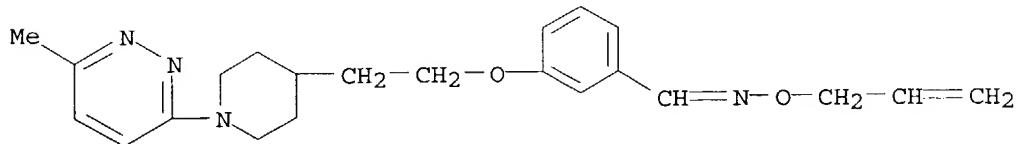
RN 314063-51-9 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



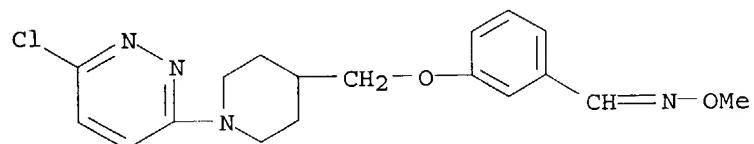
RN 314063-52-0 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



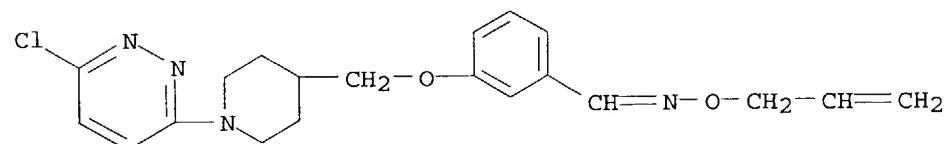
RN 314063-53-1 HCAPLUS  
 CN Benzaldehyde, 3-[(1-(6-methyl-3-pyridazinyl)-4-piperidinyl)ethoxy]-O-2-propenyloxime (9CI) (CA INDEX NAME)



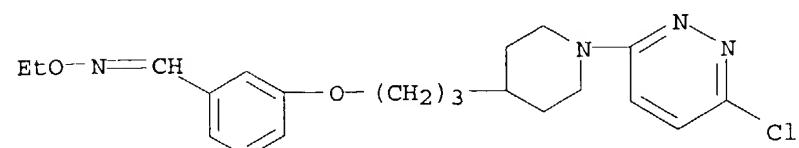
RN 314063-55-3 HCAPLUS  
 CN Benzaldehyde, 3-[(1-(6-chloro-3-pyridazinyl)-4-piperidinyl)methoxy]-O-methyloxime (9CI) (CA INDEX NAME)



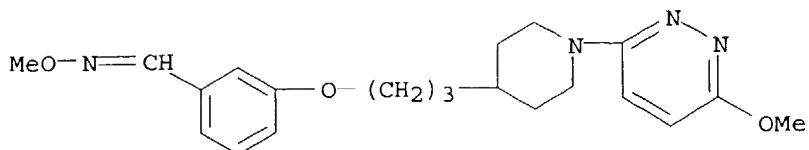
RN 314063-57-5 HCAPLUS  
 CN Benzaldehyde, 3-[(1-(6-chloro-3-pyridazinyl)-4-piperidinyl)methoxy]-O-2-propenyloxime (9CI) (CA INDEX NAME)



RN 314063-59-7 HCAPLUS  
 CN Benzaldehyde, 3-[(1-(6-chloro-3-pyridazinyl)-4-piperidinyl)propoxy]-O-ethyloxime (9CI) (CA INDEX NAME)

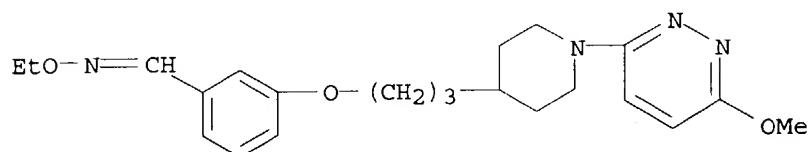


RN 314063-60-0 HCAPLUS  
 CN Benzaldehyde, 3-[(1-(6-methoxy-3-pyridazinyl)-4-piperidinyl)propoxy]-O-methyloxime (9CI) (CA INDEX NAME)



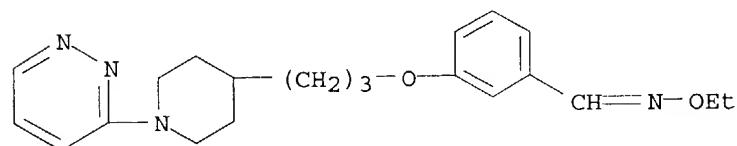
RN 314063-61-1 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



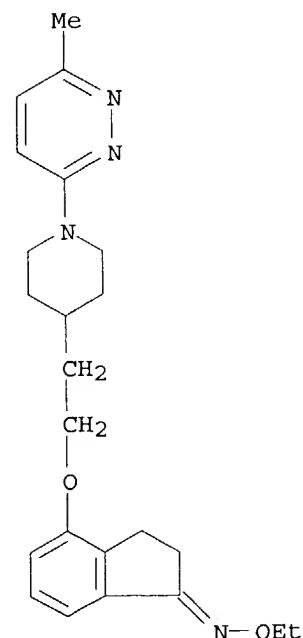
RN 314063-64-4 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



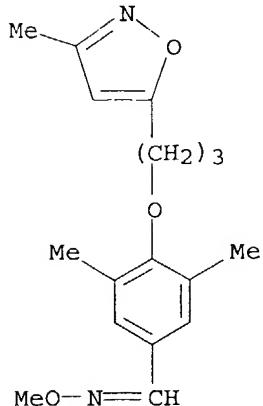
RN 314063-66-6 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



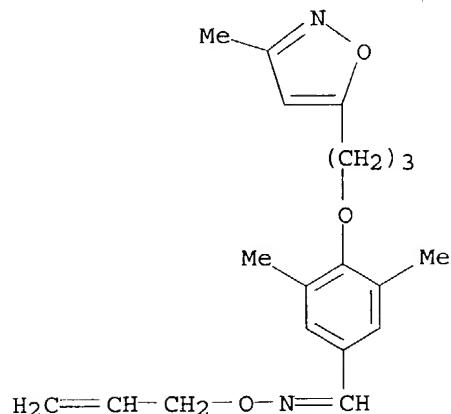
RN 314063-67-7 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



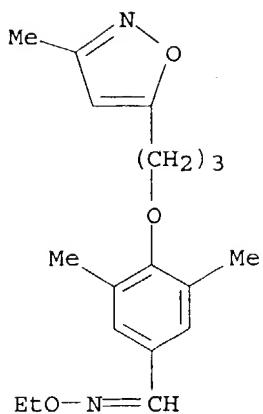
RN 314063-68-8 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



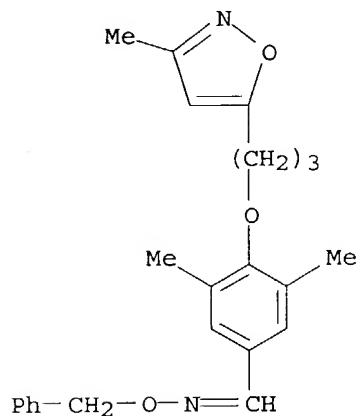
RN 314063-69-9 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



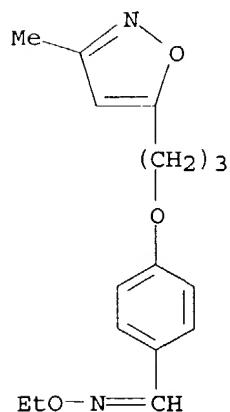
RN 314063-70-2 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(phenylmethyl)oxime (9CI) (CA INDEX NAME)



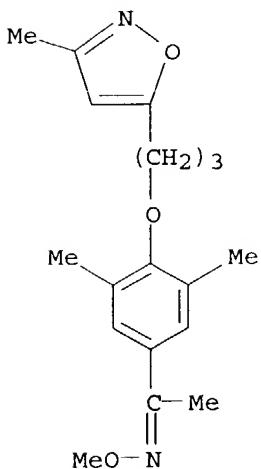
RN 314063-71-3 HCPLUS

CN Benzaldehyde, 4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



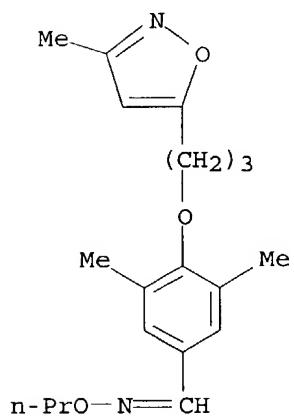
RN 314063-72-4 HCPLUS

CN Ethanone, 1-[3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)



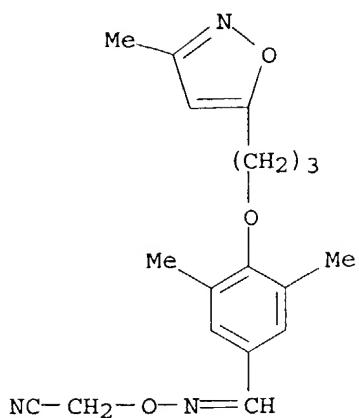
RN 314063-73-5 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-propyloxime (9CI) (CA INDEX NAME)



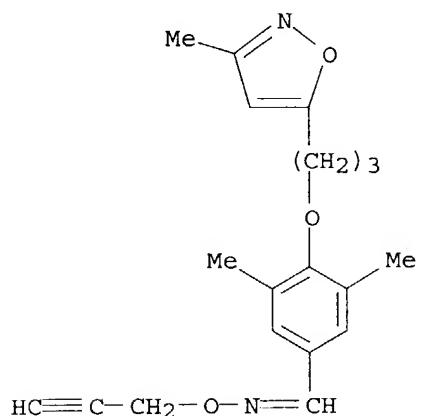
RN 314063-74-6 HCAPLUS

CN Acetonitrile, [[[3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]phenyl)methylene]amino]oxy]- (9CI) (CA INDEX NAME)



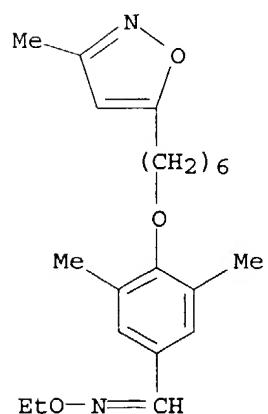
RN 314063-75-7 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-2-propynylloxime (9CI) (CA INDEX NAME)



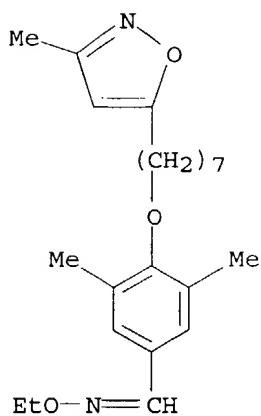
RN 314063-76-8 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[6-(3-methyl-5-isoxazolyl)hexyl]oxy-, O-ethyloxime (9CI) (CA INDEX NAME)



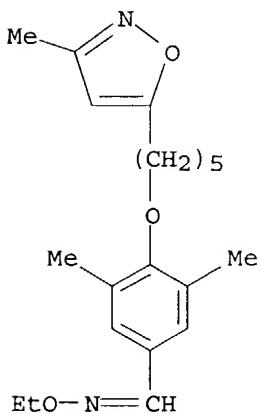
RN 314063-77-9 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[7-(3-methyl-5-isoxazolyl)heptyloxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



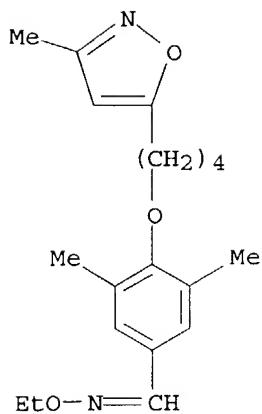
RN 314063-78-0 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[5-(3-methyl-5-isoxazolyl)pentyl]oxy-, O-ethyloxime (9CI) (CA INDEX NAME)



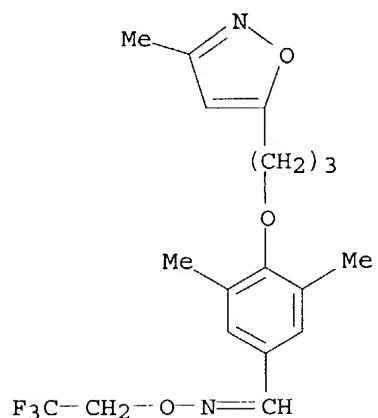
RN 314063-79-1 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[4-(3-methyl-5-isoxazolyl)butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



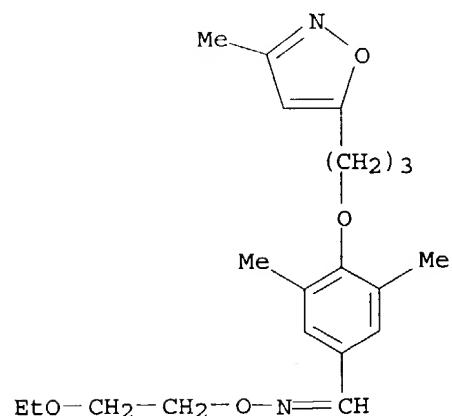
RN 314063-80-4 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2,2,2-trifluoroethyl)oxime (9CI) (CA INDEX NAME)



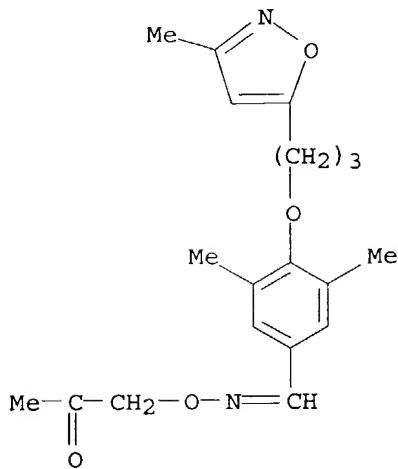
RN 314063-81-5 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-ethoxyethyl)oxime (9CI) (CA INDEX NAME)



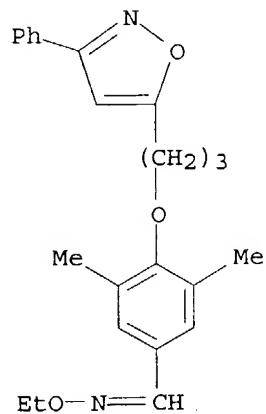
RN 314063-82-6 HCPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-oxopropyl)oxime (9CI) (CA INDEX NAME)



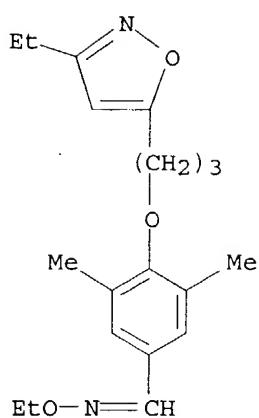
RN 314063-83-7 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-phenyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



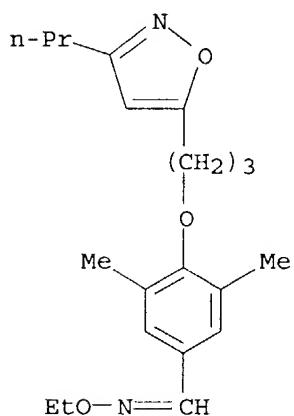
RN 314063-84-8 HCAPLUS

CN Benzaldehyde, 4-[3-(3-ethyl-5-isoxazolyl)propoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)



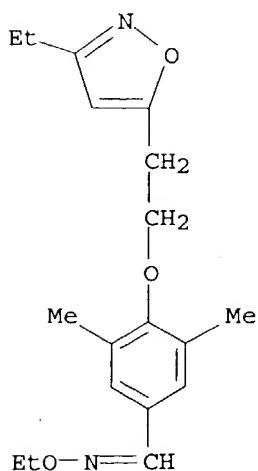
RN 314063-85-9 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-propyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



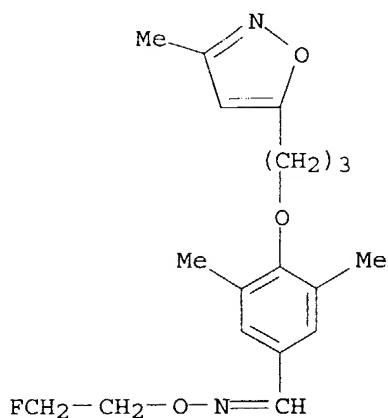
RN 314063-86-0 HCAPLUS

CN Benzaldehyde, 4-[2-(3-ethyl-5-isoxazolyl)ethoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)



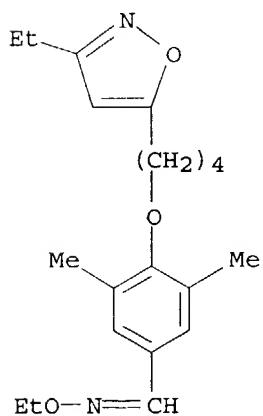
RN 314063-87-1 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-fluoroethyl)oxime (9CI) (CA INDEX NAME)



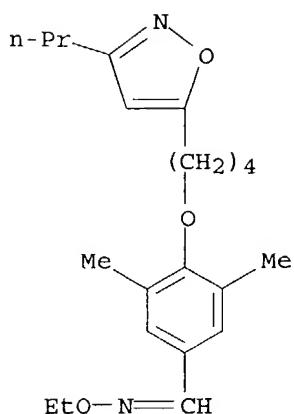
RN 314063-89-3 HCAPLUS

CN Benzaldehyde, 4-[4-(3-ethyl-5-isoxazolyl)butoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)



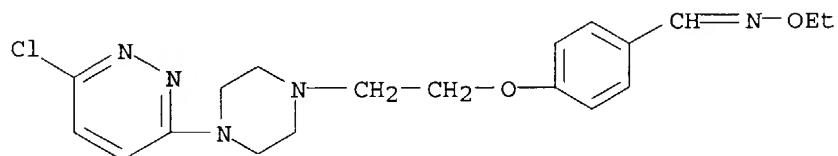
RN 314063-90-6 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[4-(3-propyl-5-isoxazolyl)butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



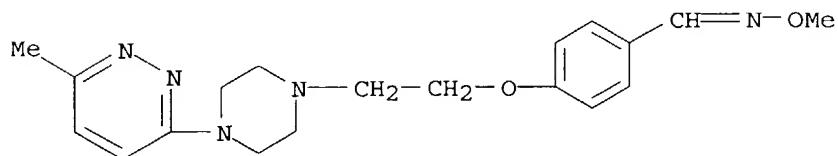
RN 314063-91-7 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



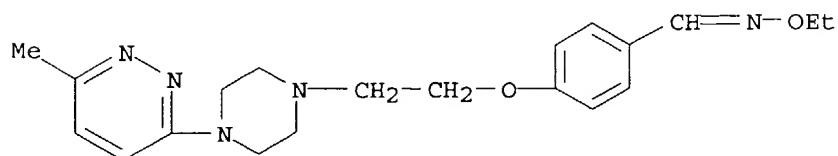
RN 314063-95-1 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



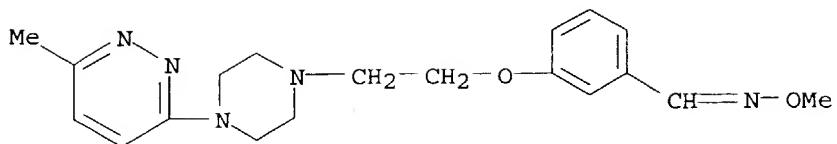
RN 314063-96-2 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

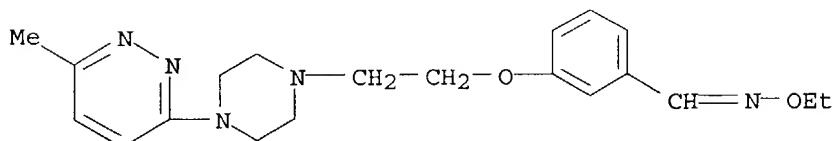


RN 314063-98-4 HCAPLUS

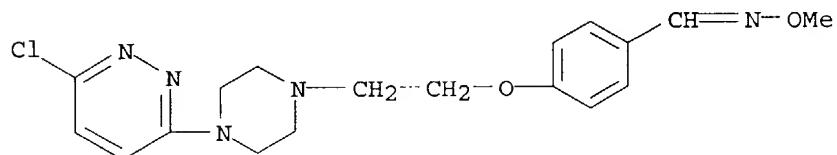
CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



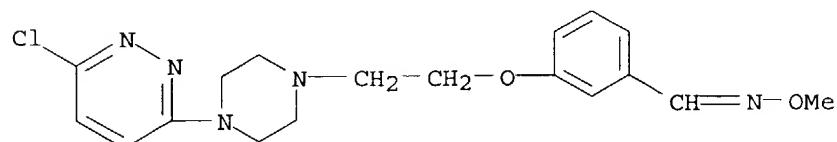
RN 314063-99-5 HCAPLUS  
 CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



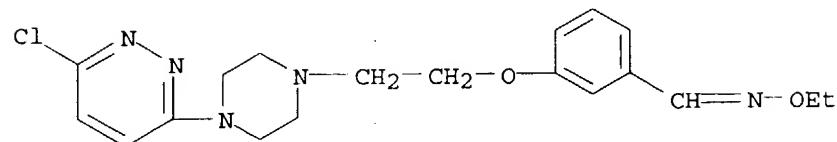
RN 314064-01-2 HCAPLUS  
 CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



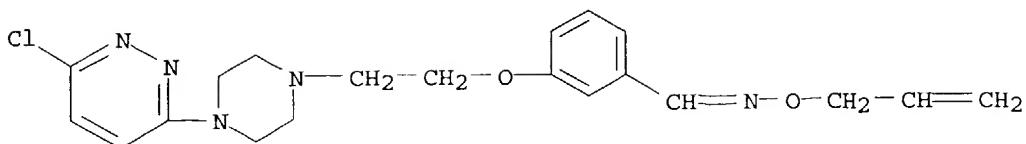
RN 314064-03-4 HCAPLUS  
 CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



RN 314064-04-5 HCAPLUS  
 CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

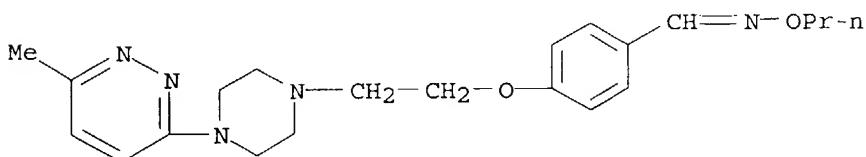


RN 314064-05-6 HCAPLUS  
 CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



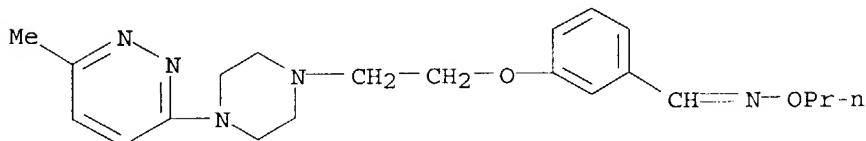
RN 314064-06-7 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-propoxime (9CI) (CA INDEX NAME)



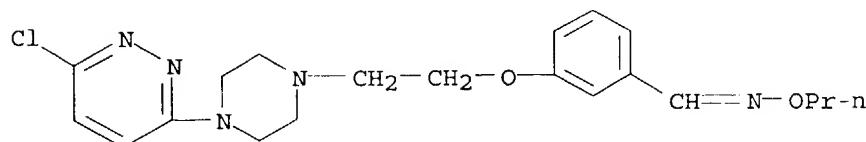
RN 314064-07-8 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-propoxime (9CI) (CA INDEX NAME)



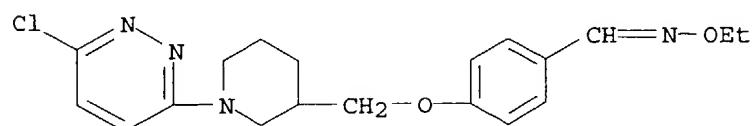
RN 314064-08-9 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-propoxime (9CI) (CA INDEX NAME)



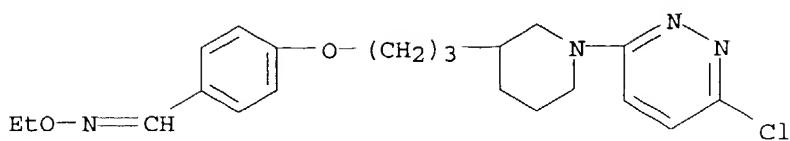
RN 314064-09-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]methoxy]-, O-ethoxime (9CI) (CA INDEX NAME)

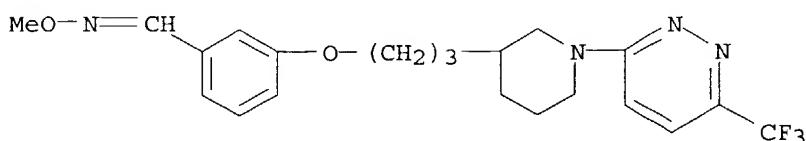


RN 314064-13-6 HCAPLUS

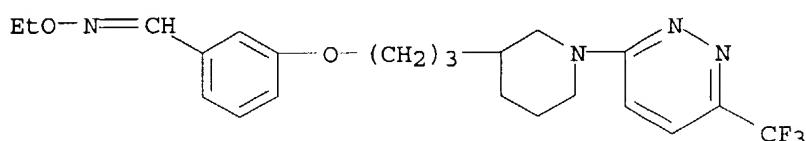
CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]propoxy]-, O-ethoxime (9CI) (CA INDEX NAME)



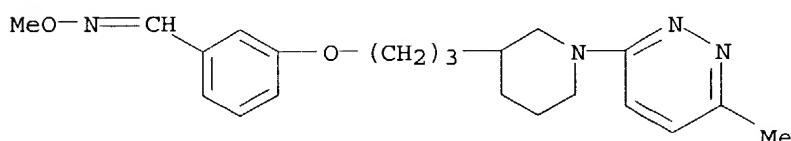
RN 314064-14-7 HCPLUS  
 CN Benzaldehyde, 3-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



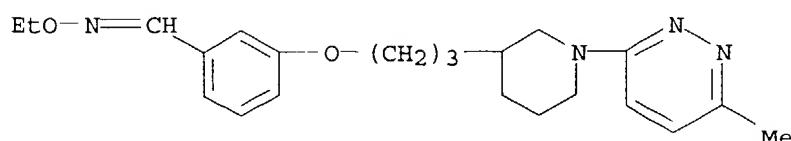
RN 314064-15-8 HCPLUS  
 CN Benzaldehyde, 3-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



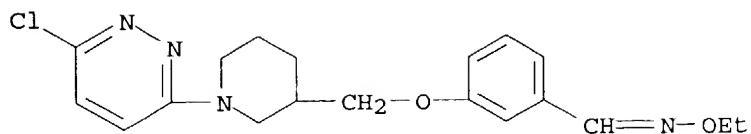
RN 314064-16-9 HCPLUS  
 CN Benzaldehyde, 3-[3-[1-(6-methyl-3-pyridazinyl)-3-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



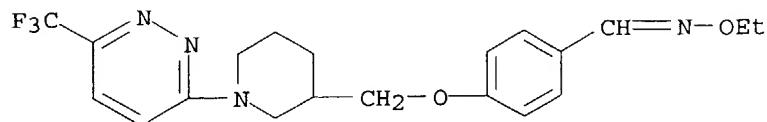
RN 314064-17-0 HCPLUS  
 CN Benzaldehyde, 3-[3-[1-(6-methyl-3-pyridazinyl)-3-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



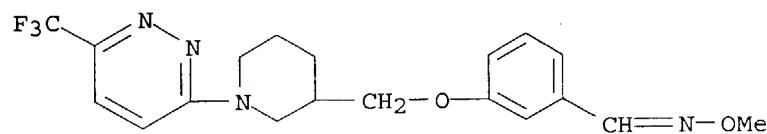
RN 314064-18-1 HCPLUS  
 CN Benzaldehyde, 3-[3-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



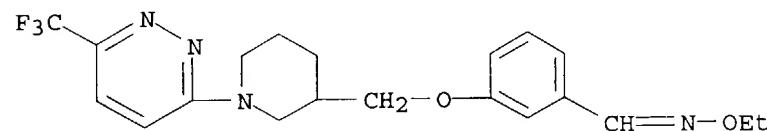
RN 314064-19-2 HCAPLUS  
 CN Benzaldehyde, 4-[(1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl)methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



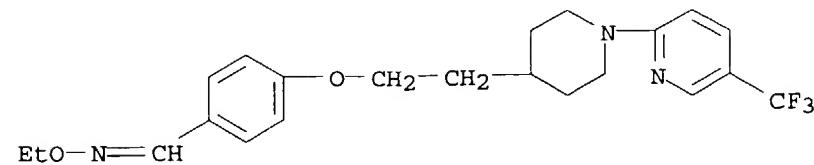
RN 314064-20-5 HCAPLUS  
 CN Benzaldehyde, 3-[(1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl)methoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



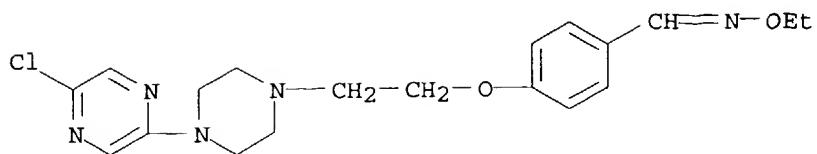
RN 314064-21-6 HCAPLUS  
 CN Benzaldehyde, 3-[(1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl)methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



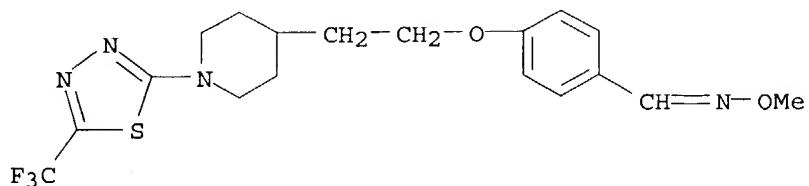
RN 314064-22-7 HCAPLUS  
 CN Benzaldehyde, 4-[(2-[(1-[6-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl)ethoxy]-4-piperidinyl)ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



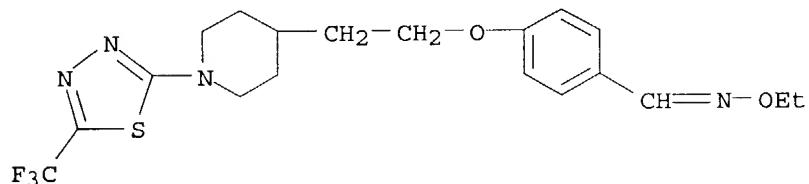
RN 314064-23-8 HCAPLUS  
 CN Benzaldehyde, 4-[(4-[(1-[6-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl)ethoxy]-4-piperidinyl)ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



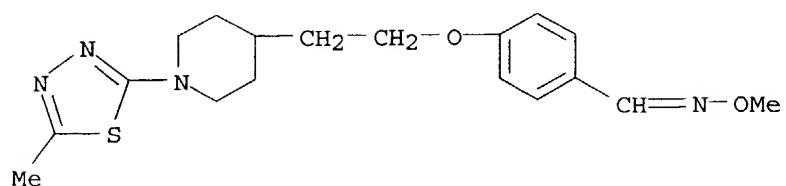
RN 314064-24-9 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



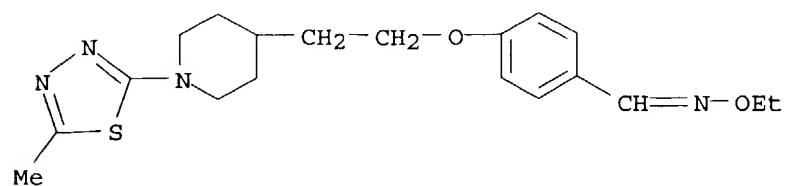
RN 314064-25-0 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314064-26-1 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(5-methyl-1,3,4-thiadiazol-2-yl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

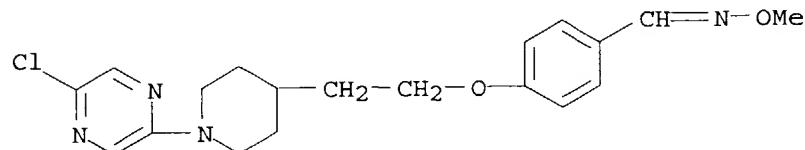


RN 314064-27-2 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(5-methyl-1,3,4-thiadiazol-2-yl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



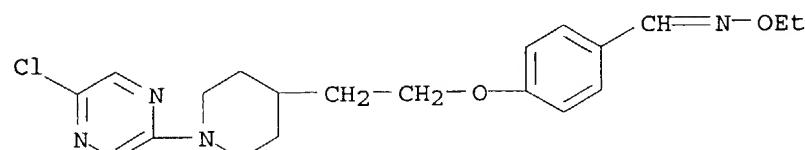
RN 314064-28-3 HCPLUS

CN Benzaldehyde, 4-[2-[1-(5-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



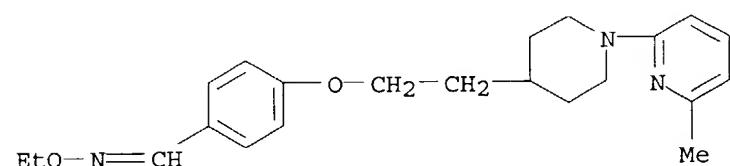
RN 314064-29-4 HCPLUS

CN Benzaldehyde, 4-[2-[1-(5-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



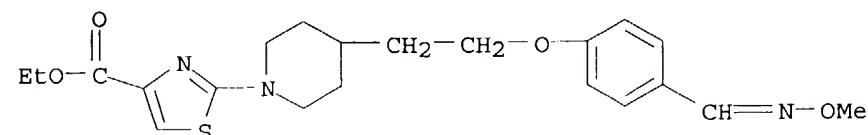
RN 314064-30-7 HCPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-2-pyridinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



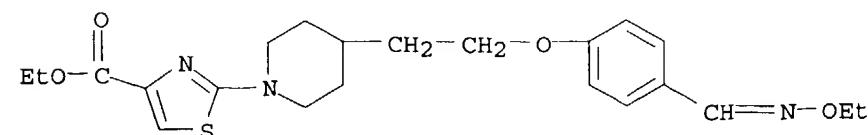
RN 314064-31-8 HCPLUS

CN 4-Thiazolecarboxylic acid, 2-[4-[2-[4-[(methoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



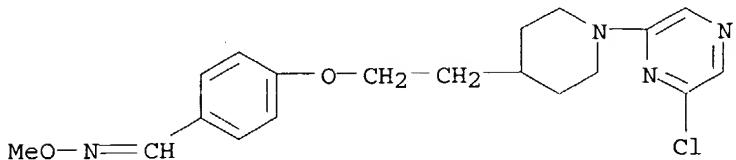
RN 314064-32-9 HCPLUS

CN 4-Thiazolecarboxylic acid, 2-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



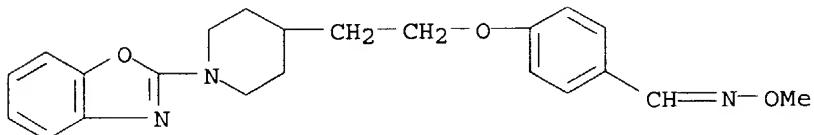
RN 314064-33-0 HCPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



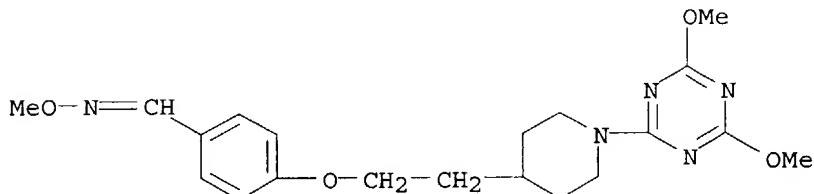
RN 314064-34-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzoxazolyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



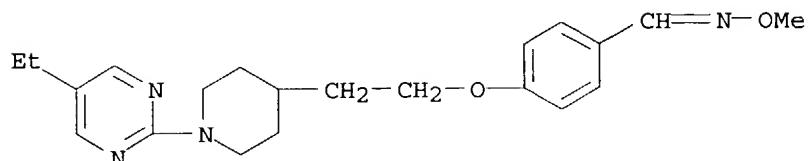
RN 314064-36-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



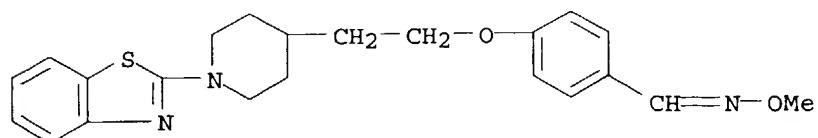
RN 314064-40-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-ethyl-2-pyrimidinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



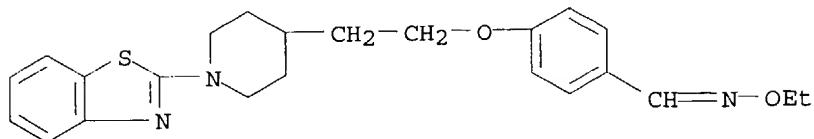
RN 314064-44-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzothiazolyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



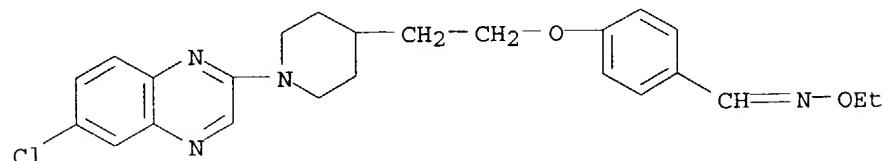
RN 314064-46-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzothiazolyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



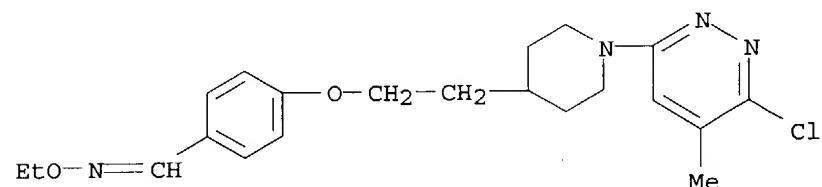
RN 314064-47-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-2-quinoxalinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



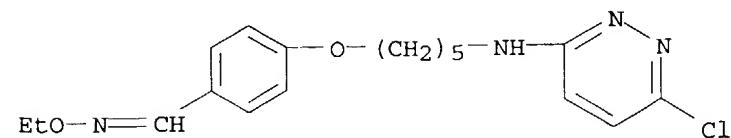
RN 314064-48-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-5-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



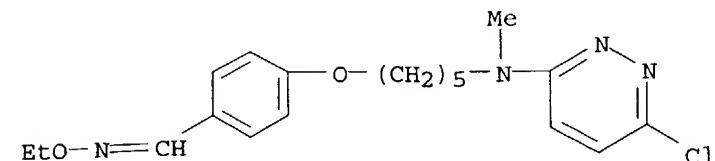
RN 314064-49-8 HCAPLUS

CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)amino]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



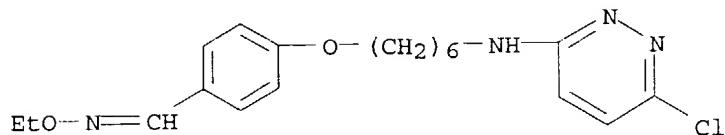
RN 314064-50-1 HCAPLUS

CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)methylamino]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



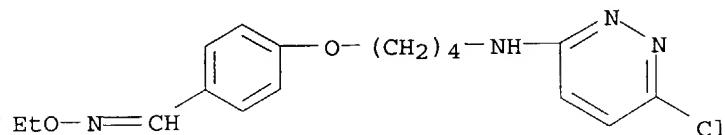
BN 314064-51-2 HCAPLUS

RN 314084-51-2 (INCI NAME)  
CN Benzaldehyde, 4-[6-[(6-chloro-3-pyridazinyl)amino]hexyl]oxy]-, Q-ethyloxime (9CI) (CA INDEX NAME)



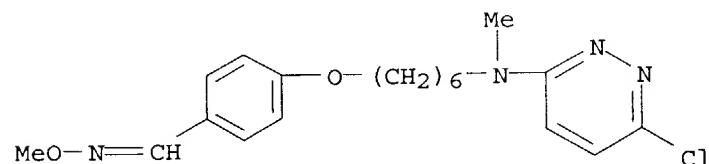
RN 314064-52-3 HCAPLUS

CN Benzaldehyde, 4-[4-[(6-chloro-3-pyridazinyl)amino]butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



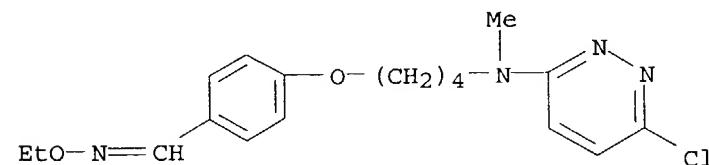
RN 314064-53-4 HCAPLUS

KN 514664-35-1 (CA INDEX NAME)  
CN Benzaldehyde, 4-[[6-[(6-chloro-3-pyridazinyl)methylamino]hexyl]oxy]-, O-methyloxime (9CI) (CA INDEX NAME)



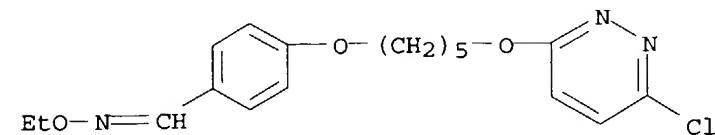
BN 314064-54-5 HCAPLUS

RN 314064-35-3 | [Chem3D](#)  
CN Benzaldehyde, 4-[4-[(6-chloro-3-pyridazinyl)methylamino]butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

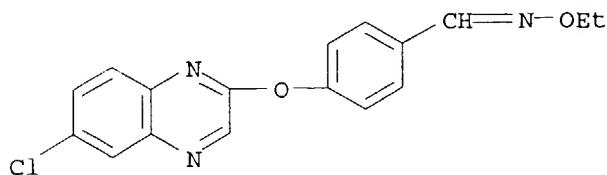


RN 314064-55-6 HCAPLUS

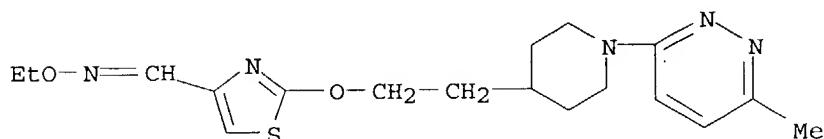
RN 314684-35-6 (INCHI) CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)oxy]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



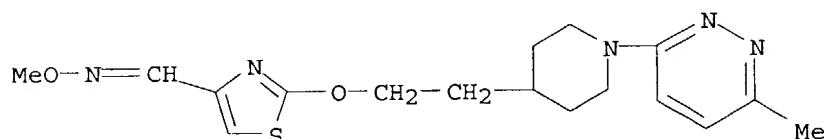
RN 314064-56-7 HCAPLUS  
 CN Benzaldehyde, 4-[(6-chloro-2-quinoxalinyloxy)-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314064-57-8 HCAPLUS  
 CN 4-Thiazolecarboxaldehyde, 2-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314064-58-9 HCAPLUS  
 CN 4-Thiazolecarboxaldehyde, 2-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

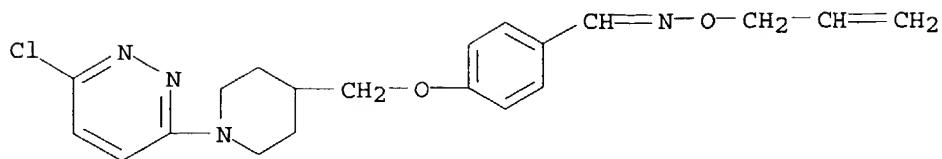


IT 314062-99-2 314063-03-1 314063-14-4  
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 314063-63-3 314063-65-5 314063-88-2  
 314063-92-8 314063-93-9 314063-94-0  
 314063-97-3 314064-00-1 314064-02-3  
 314064-10-3 314064-11-4 314064-12-5  
 314064-35-2 314064-38-5 314064-42-1  
 314255-60-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

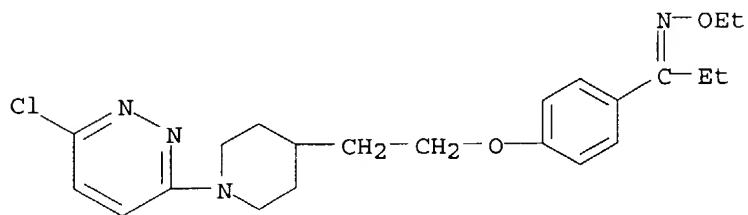
(preparation of (heterocyclalkoxy)benzaldehyde oximes as antiviral agents)

RN 314062-99-2 HCAPLUS  
 CN Benzaldehyde, 4-[(1-(6-chloro-3-pyridazinyl)-4-piperidinyl)methoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



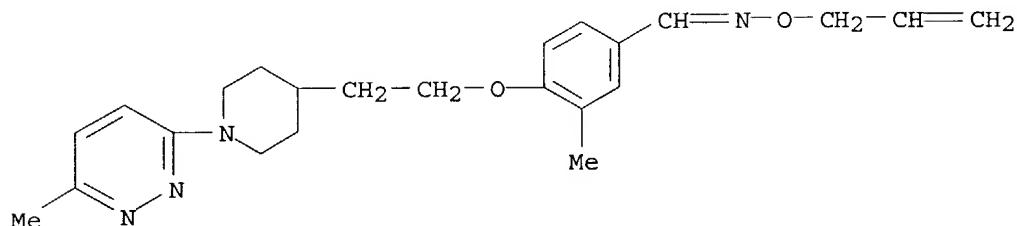
RN 314063-03-1 HCAPLUS

CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)



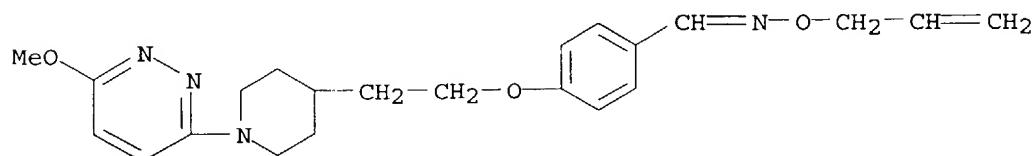
RN 314063-14-4 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenylloxime (9CI) (CA INDEX NAME)



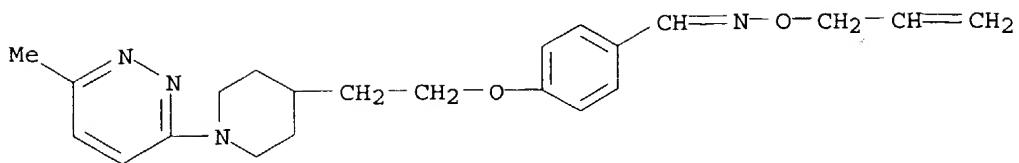
RN 314063-21-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenylloxime (9CI) (CA INDEX NAME)

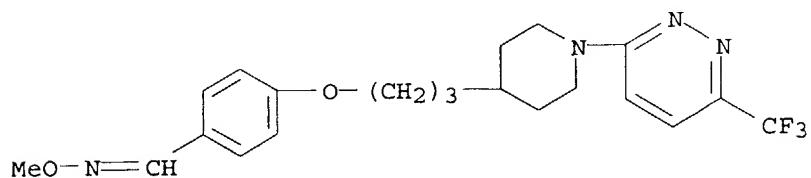


RN 314063-24-6 HCAPLUS

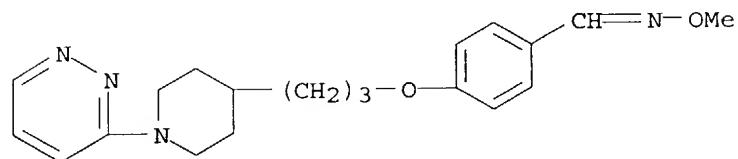
CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenylloxime (9CI) (CA INDEX NAME)



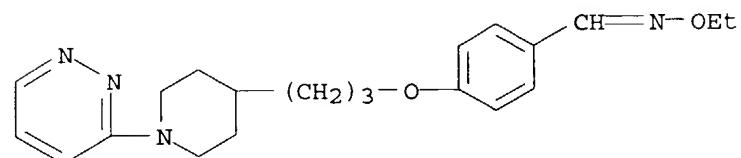
RN 314063-29-1 HCAPLUS  
 CN Benzaldehyde, 4-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



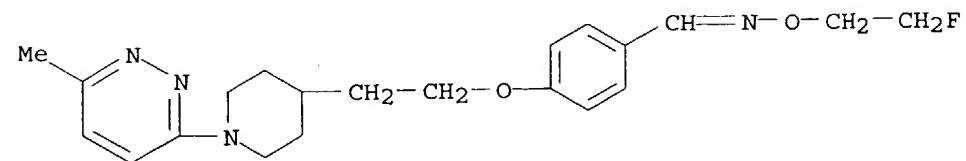
RN 314063-30-4 HCAPLUS  
 CN Benzaldehyde, 4-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



RN 314063-31-5 HCAPLUS  
 CN Benzaldehyde, 4-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

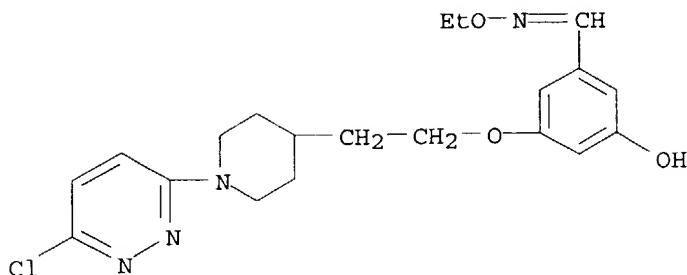


RN 314063-34-8 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2-fluoroethyl)oxime (9CI) (CA INDEX NAME)



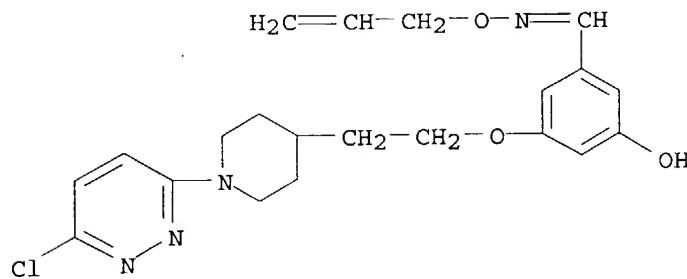
RN 314063-49-5 HCAPLUS  
 CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-

hydroxy-, O-ethyloxime (9CI) (CA INDEX NAME)



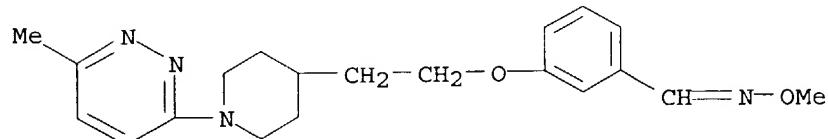
RN 314063-50-8 HCPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-hydroxy-, O-2-propenylloxime (9CI) (CA INDEX NAME)



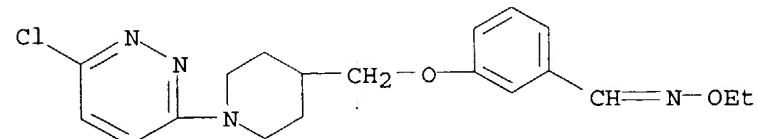
RN 314063-54-2 HCPLUS

CN Benzaldehyde, 3-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-O-methyloxime (9CI) (CA INDEX NAME)



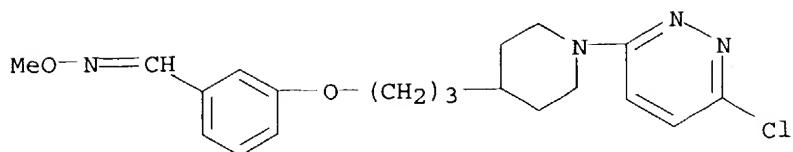
RN 314063-56-4 HCPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-O-ethyloxime (9CI) (CA INDEX NAME)

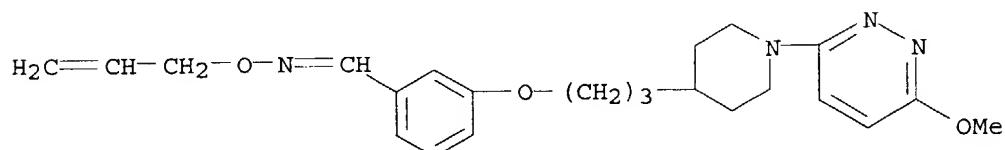


RN 314063-58-6 HCPLUS

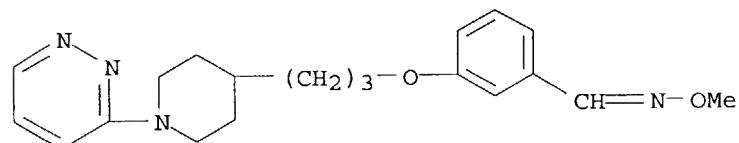
CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-O-methyloxime (9CI) (CA INDEX NAME)



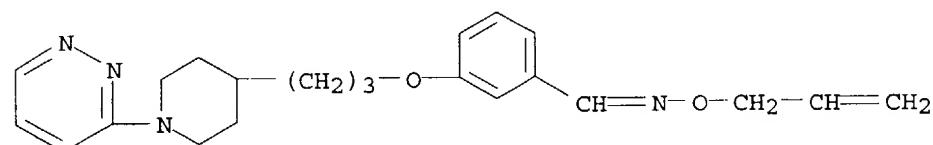
RN 314063-62-2 HCAPLUS  
 CN Benzaldehyde, 3-[3-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



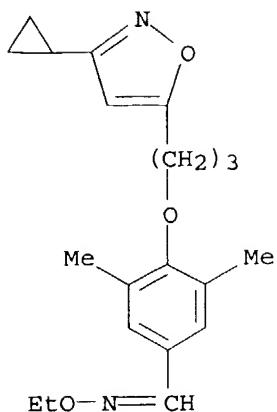
RN 314063-63-3 HCAPLUS  
 CN Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)



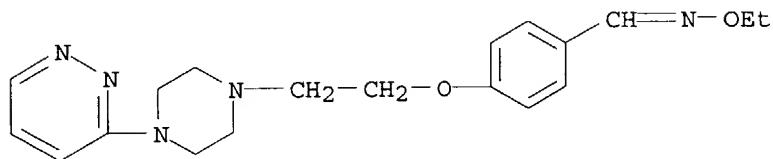
RN 314063-65-5 HCAPLUS  
 CN Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



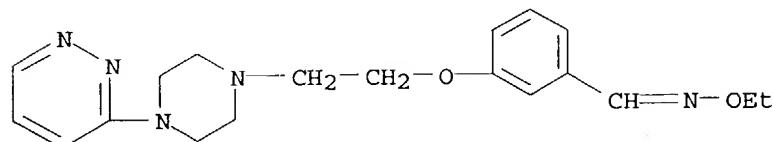
RN 314063-88-2 HCAPLUS  
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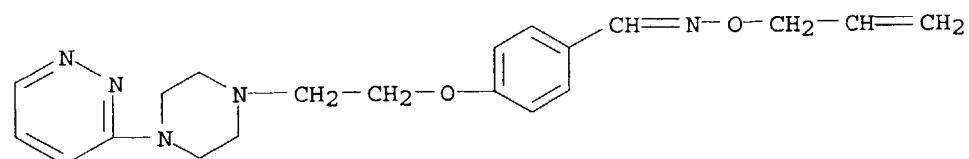
RN 314063-92-8 HCAPLUS  
 CN Benzaldehyde, 4-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime  
 (9CI) (CA INDEX NAME)



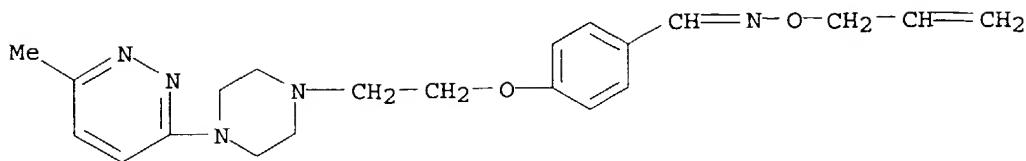
RN 314063-93-9 HCAPLUS  
 CN Benzaldehyde, 3-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime  
 (9CI) (CA INDEX NAME)



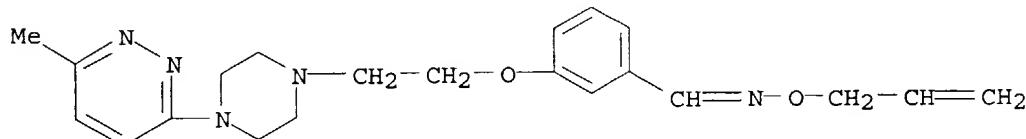
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 CN Benzaldehyde, 4-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-,  
 O-2-propenyloxime (9CI) (CA INDEX NAME)



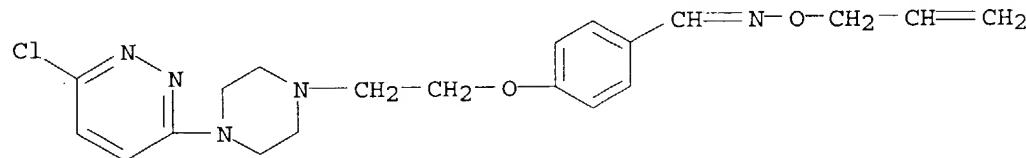
RN 314063-97-3 HCAPLUS  
 CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-,  
 O-2-propenyloxime (9CI) (CA INDEX NAME)



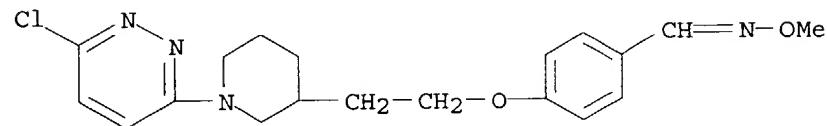
RN 314064-00-1 HCPLUS  
 CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



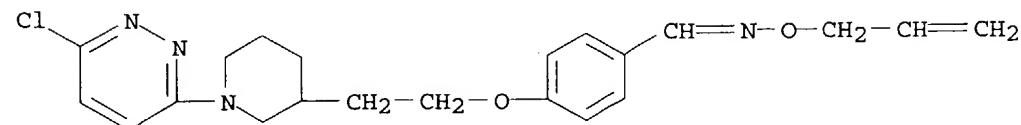
RN 314064-02-3 HCPLUS  
 CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



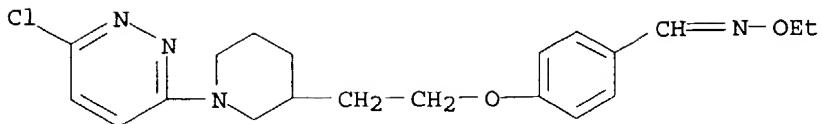
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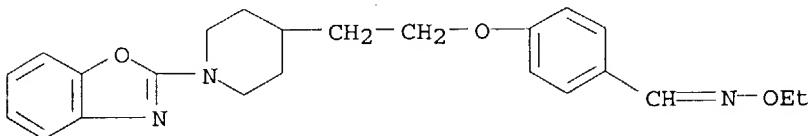
RN 314064-11-4 HCPLUS  
 CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)



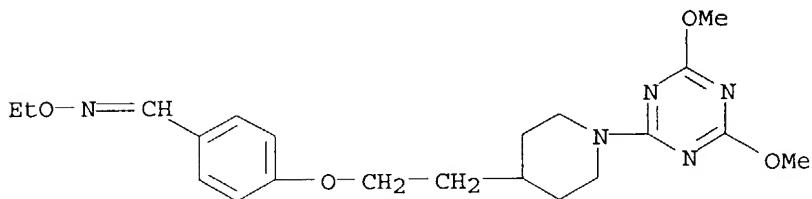
RN 314064-12-5 HCPLUS  
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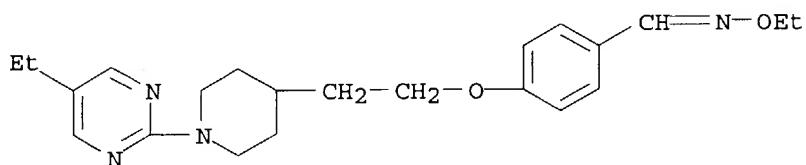
RN 314064-35-2 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(2-benzoxazolyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314064-38-5 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314064-42-1 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-(5-ethyl-2-pyrimidinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)



RN 314255-60-2 HCAPLUS  
 CN Benzaldehyde, 4-[2-[1-[6-methyloxido-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

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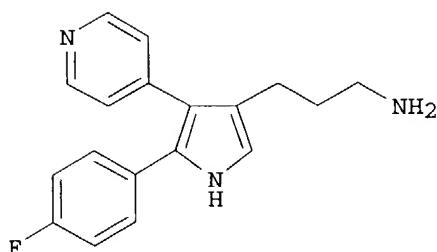
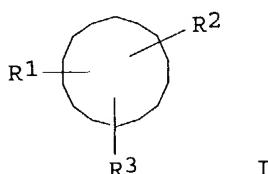
L87 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2004:220079 HCAPLUS  
 DN 140:253575  
 ED Entered STN: 19 Mar 2004  
 TI Preparation of heteroaryl-substituted pyrrole derivatives that inhibit production of TNF $\alpha$   
 IN Kimura, Tomio; Aoki, Kazumasa; Nakao, Akira; Ushiyama, Shigeru; Shimozato, Takaichi; Ohkawa, Nobuyuki; Nagasaki, Takayoshi; Yamazaki, Takanori

PA Sankyo Company, Limited, Japan  
 SO U.S. Pat. Appl. Publ., 244 pp., Cont.-in-part of U.S. Ser. No. 317,748,  
 abandoned.  
 CODEN: USXXCO  
 DT Patent  
 LA English  
 IC ICM C07D417-14  
 ICS C07D413-14; C07D043-14  
 NCL 544060000; 544141000; 544295000; 544333000; 546193000; 546269700;  
 546271400; 546272700; 546276400  
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004054173	A1	20040318	US 2003-354648	20030130 <--
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	ZA 2000003705	A	20010205	ZA 2000-3705	20000721 <--
	JP 2002284783	A2	20021003	JP 2002-12247	20020122
PRAI	JP 1999-205491	A	19990721 <--		
	JP 1999-369678	A	19991227 <--		
	US 2000-619898	B3	20000719		
	JP 2001-13817	A	20010122		
	US 2001-275005P	P	20010312		
	US 2002-54630	B2	20020122		
	US 2002-99176	B1	20020314		
	US 2002-317748	B2	20021212		

GI



AB Title compds. I [A = pyrrole; R1 = (un)substituted Ph, naphthyl, etc.; R2 = pyridinyl, pyrimidinyl, etc.; R3 = heterocyclyl] are prepared For instance,  $\alpha$ -(p-toluenesulfonyloxy)-4-fluorobenzylisonitrile is reacted with 3-(4-pyridyl)acrylate (THF, n-BuLi, LiBr,  $-45^\circ$ ) to give 4-(ethoxycarbonyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole. This Et ester is reduced (THF/PhMe, DIBAL), oxidized to the 4-formyl derivative (DMSO, MnO<sub>2</sub>, 50°), condensed with diethylphosphonoacetonitrile (THF, NaH). This adduct was reduced (THF/MeOH, H<sub>2</sub>-Pd/C) and reduced (THF, LAH) to give II. Compds. of the

invention inhibit production of TNF $\alpha$  and IL-1 $\beta$ . They are useful for the treatment of inflammation.

ST heteroaryl pyrrole pyridine pyrimidine TNF interleukin inhibitor prepn

IT Intestine, disease  
(Crohn's; preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Bone  
(absorption, inhibition of; preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Heart, disease  
(ischemia; preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Kidney, disease  
(nephritis; preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Allergy inhibitors

Alzheimer's disease

Analgesics

Anti-Alzheimer's agents

Anti-inflammatory agents

Antiarteriosclerotics

Antiarthritics

Antidiabetic agents

Antirheumatic agents

Antiviral agents

Arteriosclerosis

Diabetes mellitus

Fever and Hyperthermia

Hepatitis

Human

Lupus erythematosus

Osteoarthritis

Osteoporosis

Pain

Psoriasis

Rheumatoid arthritis

Septicemia  
(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Cytokines

Interleukin 1 $\beta$

Tumor necrosis factors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT Intestine, disease  
(ulcerative colitis; preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT 321344-57-4P 321344-58-5P  
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT 321343-74-2P, 4-(3-Aminopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321343-78-6P, 4-Aminomethyl-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole Dihydrochloride 321343-82-2P, 4-(1-Acetyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321343-83-3P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-tetrahydropyridin-4-yl)-1H-pyrrole dihydrochloride 321343-86-6P,

1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole  
 321343-87-7P, 3-(4-Fluorophenyl)-1-(piperidin-4-yl)-2-(pyridin-4-yl)-1H-pyrrole  
 321343-98-0P 321344-06-3P, 2-(4-Fluorophenyl)-4-(1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-09-6P  
 321344-17-6P, 2-(4-Fluorophenyl)-4-(8-methyl-8-azabicyclo[3.2.1]oct-2-en-3-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-19-8P, 4-(8-Azabicyclo[3.2.1]oct-2-en-3-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-21-2P,  
 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-tetrahydro-2,2,6,6-tetramethylpyridin-4-yl)-1H-pyrrole 321344-24-5P, 2-(4-Fluorophenyl)-4-(6-methyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-26-7P 321344-28-9P, 2-(4-Fluorophenyl)-4-(1-isopropyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-33-6P,  
 2-(4-Fluorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-34-7P, 2-(4-Fluorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-37-0P,  
 2-(4-Fluorophenyl)-4-(1,2,2,6,6-pentamethyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heteroaryl-substituted pyrrole derivs. that inhibit

production

of TNF $\alpha$ )

IT 321343-75-3P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(3-trifluoroacetylaminopropyl)-1H-pyrrole 321343-76-4P,  
 4-(3-Acetylaminopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321343-77-5P, 2-(4-Fluorophenyl)-4-(3-methylaminopropyl)-3-(pyridin-4-yl)-1H-pyrrole 321343-79-7P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(2,4,6-trifluorobenzoylaminomethyl)-1H-pyrrole 321343-80-0P,  
 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(2,3,5,6-tetrafluoropyridin-4-yl)-1H-pyrrole 321343-81-1P, [5-(4-Fluorophenyl)-4-(pyridin-4-yl)-1H-pyrrol-3-yl](pyridin-4-yl)methanol 321343-84-4P, 2-(4-Fluorophenyl)-4-(piperidin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321343-88-8P, 3-(4-Fluorophenyl)-1-(1-methylpiperidin-4-yl)-2-(pyridin-4-yl)-1H-pyrrole 321343-89-9P,  
 1-(1-Acetylaminopropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole  
 321343-90-2P, 3-(4-Fluorophenyl)-1-[1-(2-nitroethyl)piperidin-4-yl]-2-(pyridin-4-yl)-1H-pyrrole 321343-92-4P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-(pyrrolidin-3-yl)-1H-pyrrole 321343-93-5P, 3-(4-Fluorophenyl)-1-(piperidin-3-yl)-2-(pyridin-4-yl)-1H-pyrrole 321343-94-6P,  
 3-(4-Fluorophenyl)-1-(piperidin-4-yl)methyl-2-(pyridin-4-yl)-1H-pyrrole  
 321343-95-7P, 1-(Azetidin-3-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole dihydrochloride 321343-96-8P, 1-(3-Aminopropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321343-97-9P,  
 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-[3-(thiomorpholinyl)propyl]-1H-pyrrole 321343-99-1P, 2-(4-Fluorophenyl)-4-[3-(piperazin-1-yl)propyl]-3-(pyridin-4-yl)-1H-pyrrole 321344-00-7P, 4-(3-Dimethylaminopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-01-8P,  
 2-(4-Fluorophenyl)-4-[3-(morpholinyl)propyl]-3-(pyridin-4-yl)-1H-pyrrole 321344-02-9P, 2-(4-Fluorophenyl)-4-[3-(piperidin-1-yl)propyl]-3-(pyridin-4-yl)-1H-pyrrole 321344-03-0P, 2-(4-Fluorophenyl)-4-[3-(1-methylpiperazin-4-yl)propyl]-3-(pyridin-4-yl)-1H-pyrrole 321344-04-1P,  
 1-(3-Dimethylaminopropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole  
 321344-05-2P, 2-(4-Fluorophenyl)-3,4-bis(pyridin-4-yl)-1H-pyrrole  
 321344-07-4P, 2-(4-Fluorophenyl)-4-(1-methylpiperidin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-08-5P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-(2,2,6,6-tetramethylpiperidin-4-yl)-1H-pyrrole 321344-10-9P,  
 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(quinuclidin-3-yl)-1H-pyrrole  
 321344-11-0P, 2-(4-Fluorophenyl)-4-(4-hydroxypiperidin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-12-1P, 2-(4-Fluorophenyl)-4-(3-((methanesulfonyl)amino)propyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-13-2P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-(quinuclidin-3-yl)-1H-pyrrole 321344-14-3P, 3-(4-Fluorophenyl)-1-(piperidin-3-yl)methyl-2-(pyridin-4-yl)-1H-pyrrole 321344-15-4P, cis-1-(4-Aminocyclohexyl)-3-(4-

fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-16-5P,  
 3-(4-Fluorophenyl)-2-(2-methylaminopyrimidin-4-yl)-1-(piperidin-4-yl)-1H-  
 pyrrole 321344-18-7P, 2-(4-Fluorophenyl)-4-(8-methyl-8-  
 azabicyclo[3.2.1]octan-3-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-20-1P,  
 4-(8-Azabicyclo[3.2.1]octan-3-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-  
 pyrrole 321344-22-3P, 2-(4-Fluorophenyl)-3-(Pyridin-4-yl)-4-(2,2,6,6-  
 tetramethylpiperidin-4-yl)-1H-pyrrole 321344-23-4P, 2-(4-Fluorophenyl)-4-  
 (2-methyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-25-6P, 2-(4-Fluorophenyl)-4-(2-methylpiperidin-4-yl)-3-(pyridin-4-  
 yl)-1H-pyrrole 321344-27-8P, 4-(1-Ethylpiperidin-4-yl)-2-(4-  
 fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-29-0P,  
 2-(4-Fluorophenyl)-4-(1-isopropylpiperidin-4-yl)-3-(pyridin-4-yl)-1H-  
 pyrrole 321344-30-3P, 2-(4-Fluorophenyl)-4-(1-propyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-31-4P,  
 4-(1-Benzyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-  
 4-yl)-1H-pyrrole 321344-32-5P, 2-(4-Fluorophenyl)-4-(1-phenethyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-35-8P,  
 4-(1,6-Dimethyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-  
 (pyridin-4-yl)-1H-pyrrole 321344-36-9P, 4-(1,2-Dimethyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-38-1P, 2-(4-Fluorophenyl)-4-(1,2,2,6,6-pentamethylpiperidin-4-yl)-3-  
 (pyridin-4-yl)-1H-pyrrole 321344-39-2P, 2-(4-Fluorophenyl)-3-(pyridin-4-  
 yl)-4-(1,2,3,6-tetrahydropyridin-5-yl)-1H-pyrrole 321344-41-6P,  
 4-(4-Aminobutyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-42-7P, 1-(2-Dimethylaminoethyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-  
 1H-pyrrole 321344-43-8P, 1-(2,2-Dimethyl-3-dimethylaminopropyl)-3-(4-  
 fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-44-9P,  
 1-(8-Azabicyclo[3.2.1]octan-3-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-  
 pyrrole 321344-45-0P, 3-(4-Fluorophenyl)-1-(2-methylpiperidin-4-yl)-2-  
 (pyridin-4-yl)-1H-pyrrole 321344-46-1P, 3-(4-Fluorophenyl)-2-(2-  
 methylaminopyridin-4-yl)-1-(piperidin-4-yl)-1H-pyrrole 321344-47-2P,  
 2-(4-Fluorophenyl)-3-[2-((1S)-1-phenylethylamino)pyridin-4-yl]-4-(1,2,3,6-  
 tetrahydropyridin-4-yl)-1H-pyrrole 321344-48-3P, 4-(1-tert-Butyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-49-4P, 2-(4-Fluorophenyl)-4-(1-octyl-1,2,3,6-tetrahydropyridin-4-  
 yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-50-7P, 4-(1-Ethyl-6-methyl-  
 1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-  
 pyrrole 321344-51-8P, 4-(1-Ethyl-2-methyl-1,2,3,6-tetrahydropyridin-4-  
 yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-52-9P,  
 2-(4-Fluorophenyl)-4-(1,2,3,5,6,7,8,8a-octahydroindolin-7-yl)-3-(pyridin-  
 4-yl)-1H-pyrrole 321344-53-0P, 4-(6-Allyl-1-methyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-54-1P, 4-(2-Allyl-1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-  
 fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-55-2P,  
 4-(6-Benzyl-1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-  
 (pyridin-4-yl)-1H-pyrrole 321344-56-3P, 4-(2-Benzyl-1-methyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-59-6P, 2-(4-Fluorophenyl)-4-(6-methyl-1-propyl-1,2,3,6-  
 tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-61-0P,  
 2-(4-Fluorophenyl)-4-(2-methyl-1-propyl-1,2,3,6-tetrahydropyridin-4-yl)-3-  
 (pyridin-4-yl)-1H-pyrrole 321344-62-1P, 2-(4-Fluorophenyl)-4-  
 (1,3,4,6,7,9a-hexahydro-2H-quinolizin-8-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-63-2P, 2-(4-Fluorophenyl)-4-(1,3,4,6,9,9a-hexahydro-2H-quinolizin-8-  
 yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-64-3P, 2-(4-Fluorophenyl)-4-  
 (1,2,3,5,8,8a-hexahydroindolin-7-yl)-3-(2-methylaminopyrimidin-4-yl)-1H-  
 pyrrole 321344-65-4P, 2-(4-Fluorophenyl)-4-(1,2,3,5,6,8a-  
 hexahydroindolin-7-yl)-3-(2-methylaminopyrimidin-4-yl)-1H-pyrrole  
 321344-66-5P, 2-(3,4-Difluorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolin-7-  
 yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-67-6P, 2-(3,4-Difluorophenyl)-4-  
 (1,2,3,5,6,8a-hexahydroindolin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 321344-68-7P, 4-(1,2,3,5,8,8a-Hexahydroindolin-7-yl)-3-(pyridin-4-yl)-2-  
 (3-trifluoromethylphenyl)-1H-pyrrole 321344-69-8P, 4-(1,2,3,5,6,8a-  
 Hexahydroindolin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-

pyrrole 321344-70-1P, 2-(3-Fluorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-71-2P,  
 2-(3-Fluorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-72-3P, 2-(3-Chlorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-73-4P,  
 2-(3-Chlorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-74-5P, 4-(1,2,3,5,8,8a-Hexahydroindolizin-7-yl)-2-phenyl-3-(pyridin-4-yl)-1H-pyrrole 321344-75-6P, 4-(1,2,3,5,6,8a-Hexahydroindolizin-7-yl)-2-phenyl-3-(pyridin-4-yl)-1H-pyrrole  
 321344-76-7P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-tetrahydropyridin-4-yl)-1H-pyrrole 443912-03-6P 443912-04-7P,  
 4-(3-Dimethylamino-1-propen-1-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 443982-89-6P 443982-91-0P 443982-92-1P 443982-94-3P  
 443982-95-4P 443982-97-6P 443983-00-4P 443983-02-6P,  
 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(6,9,9a,10-tetrahydropyrido[1,2-a]indol-8-yl)-1H-pyrrole 443983-04-8P 443983-07-1P 443983-09-3P  
 443983-13-9P 443983-15-1P 443983-17-3P 443983-19-5P 443983-21-9P  
 443983-22-0P 443983-26-4P 443983-29-7P 443983-30-0P 443983-32-2P  
 443983-33-3P 443983-34-4P, 4-(2,2-Diphenyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 443983-35-5P 443983-37-7P 443983-39-9P 443983-40-2P 443983-41-3P  
 443983-43-5P 443983-44-6P 443983-46-8P 443983-48-0P 443983-49-1P  
 443983-51-5P 443983-52-6P 443983-54-8P 443983-58-2P 443983-61-7P  
 443983-64-0P 443983-65-1P 443983-67-3P 443983-68-4P 443983-69-5P  
 443983-70-8P 443983-72-0P 443983-75-3P 443983-78-6P 443983-80-0P  
 443983-82-2P 443983-84-4P 443984-43-8P, 2-(3-Fluorophenyl)-4-(2-methyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-44-9P, 2-(3-Fluorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-45-0P,  
 2-(3-Fluorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-46-1P, 2-(4-Fluorophenyl)-4-(2-methyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-47-2P, 2-(4-Fluorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-48-3P,  
 2-(4-Fluorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-49-4P, 2-(3-Chlorophenyl)-4-(2-methyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-50-7P, 2-(3-Chlorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-51-8P,  
 4-(2-Methyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 443984-52-9P, 4-(2-Phenyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 443984-53-0P, 4-(2-Methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 443984-54-1P,  
 2-(4-Fluorophenyl)-4-(2-methyl-3,5,6,8a-tetrahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-55-2P, 2-(4-Fluorophenyl)-4-(2-methylidene-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-56-3P, 4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 443984-57-4P,  
 4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-2-(3-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 443984-58-5P, 2-(3-Chlorophenyl)-4-(2-ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-59-6P, 4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 443984-60-9P,  
 2-(4-Fluorophenyl)-4-(2-propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-61-0P, 2-(3-Fluorophenyl)-4-(2-propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-62-1P, 2-(3-Chlorophenyl)-4-(2-propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-63-2P,  
 4-(2-Propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 443984-64-3P, 4-(2-Ethyl-3,5,6,8a-tetrahydroindolizin-7-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-65-4P, 2-(4-Fluorophenyl)-4-(2-propyl-3,5,6,8a-tetrahydroindolizin-

7-yl)-3-(pyridin-4-yl)-1H-pyrrole 443984-66-5P, 2-(4-Fluorophenyl)-4-(2-phenyl-3,5,6,8a-tetrahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 443984-68-7P, 2-(4-Fluorophenyl)-3-(Pyridin-4-yl)-4-(6,7,9a,10-tetrahydropyrido[1,2-a]indol-8-yl)-1H-pyrrole 471864-21-8P  
 476487-12-4P 476487-13-5P 670274-00-7P, 4-(1,2,3,5,6,8a-Hexahydroindolizin-7-yl)-2-phenyl-3-(pyrazin-4-yl)-1H-pyrrole  
 670274-08-5P, 2-(3-Chlorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

IT 78-94-4, Methyl vinyl ketone, reactions 105-36-2, Ethyl bromoacetate 108-00-9, 2-Dimethylaminoethylamine 109-01-3, 1-Methylpiperazine 109-55-7, 3-Dimethylaminopropylamine 109-65-9, Butyl bromide 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 123-00-2, 4-(3-Aminopropyl)morpholine 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine 501-53-1, Benzyl chloroformate 532-24-1, 8-Methyl-8-azabicyclo[3.2.1]octan-3-one 700-16-3, Pentafluoropyridine 826-36-8, 2,2,6,6-Tetramethylpiperidin-4-one 867-13-0, Ethyl diethylphosphonoacetate 872-85-5, 4-Formylpyridine 1074-68-6, 4-Formyl-2-methylthiopyrimidine 1445-73-4, 1-Methylpiperidin-4-one 1449-46-3, Benzyltriphenylphosphonium bromide 1465-76-5, 1-tert-Butylpiperidin-4-one 2032-35-1, Bromoacetaldehyde diethyl acetal 2407-99-0, 1,2,3,5,6,7,8,8a-Octahydroindolizin-7-one 2537-48-6, Diethylphosphonoacetonitrile 2627-86-3, (S)-1-Phenylethylamine 2759-28-6, 1-Benzylpiperazine 3612-18-8, 1-Ethylpiperidin-4-one 3612-20-2, 1-Benzylpiperidin-4-one 3731-38-2, Quinuclidin-3-one 4124-41-8, p-Toluenesulfonic anhydride 4254-02-8, Cyclopentanecarbonitrile 5355-68-0, 1-Isopropylpiperidin-4-one 5554-54-1, 1,2,2,6,6-Pentamethylpiperidin-4-one 6238-14-8, 3-Aminoquinuclidine 13669-32-4, 1,2-Dimethylpiperidin-4-one 16217-15-5, (S)-1-Benzylloxycarbonyl-4-oxoproline methyl ester 16217-17-7 16728-64-6, 3-Benzyl oxypropylamine 18942-89-7, 2-Nitroethyl acetate 21823-56-3, 2-Benzyl-1-methylpiperidin-4-one 23133-37-1, 1-Propylpiperidin-4-one 23581-42-2, Octahydro-2H-quinolizin-2-one 24489-96-1, Ethyl 3-(4-pyridyl)acrylate 24654-55-5, 3-(4-Fluorophenyl)acrolein 28957-72-4, 8-Benzyl-8-azabicyclo[3.2.1]octan-3-one 33329-70-3, 1-Ethoxycarbonyl-1-formylcyclopropane 36635-66-2 36768-62-4, 4-Amino-2,2,6,6-tetramethylpiperidine 37517-81-0, Methyl malonyl chloride 39742-60-4, 1-Phenethylpiperidin-4-one 40114-49-6, 1-Benzylpiperidin-3-one 40432-52-8, 3-Amino-1-(diphenylmethyl)azetidine 50541-93-0, 4-Amino-1-benzylpiperidine 53369-71-4, 2,2-Dimethyl-3-dimethylaminopropylamine 64187-48-0, (2S,4R)-1-Benzylloxycarbonyl-4-hydroxypyrrrolidin-2-carboxylic acid methyl ester 71072-32-7, 1-Octylpiperidin-4-one 72180-27-9, (2S)-1-Benzylloxycarbonyl-4,4-difluoroproline 75776-70-4 79538-29-7, 2,4,6-Trifluorobenzoyl chloride 96522-37-1, (2S,4R)-1-Benzylloxycarbonyl-4-methoxypyrrrolidin-2-carboxylic acid 96901-92-7, 3-Amino-8-benzyl-8-azabicyclo[3.2.1]octane 113490-82-7 115031-85-1, 2,2-Diphenyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 131747-69-8, 2-Fluoropyridine-4-carboxaldehyde 135829-03-7, Methyl 1-benzylloxycarbonylindoline-2-carboxylate 144222-22-0, 4-Aminomethyl-1-(tert-butoxycarbonyl)piperidine 153290-87-0, (2S,4R)-1-Benzylloxycarbonyl-4-ethoxypyrrrolidin-2-carboxylic acid 156088-46-9, (S)-4,4-Dimethyl-2-hydroxymethyl-5-oxopyrrrolidine 162167-97-7, 3-Aminomethyl-1-(tert-butoxycarbonyl)piperidine 165806-95-1,  $\alpha$ -(p-Toluenesulfonyl)-4-fluorobenzylisonitrile 184637-48-7, 3-Amino-1-(tert-butoxycarbonyl)piperidine 185212-91-3 186550-13-0, 3-Amino-1-(tert-butoxycarbonyl)pyrrolidine 190906-83-3, 2-Methyl-1-propylpiperidin-4-one 203661-73-8, 1-Benzyl-2-methylpiperidin-4-one 247570-24-7, cis-4-((tert-Butoxycarbonyl)amino)cyclohexane-1-amine

263389-45-3 288620-86-0, (2S,4R)-1-Benzylloxycarbonyl-4-hydroxypiperidin-2-carboxylic acid benzyl ester 306296-67-3, 1-Allyloxycarbonylpiperidin-4-one 321344-85-8 321345-30-6, 4-Amino-1-benzyl-2-methylpiperidine 321345-31-7, Ethyl 3-(2-fluoropyridin-4-yl)acrylate 321345-32-8, 1-Ethyl-2-methylpiperidin-4-one 321345-33-9, 2-Allyl-1-methylpiperidin-4-one 321345-34-0, Ethyl 3-(2-methylthiopyrimidin-4-yl)acrylate 321345-35-1 321345-36-2 321345-37-3 443983-92-4, 2-(3-Ethoxycarbonyl-2-oxopropyl)indoline 443983-94-6, Methyl (S)-1-benzylloxycarbonyl-4-phenyl-3-pyrroline-2-carboxylate 443984-09-6, (2S,4S)-4-Methoxypiperidin-2-carboxylic acid hydrochloride 443984-25-6, (S)-1-(Benzylloxycarbonyl)piperidin-2-carboxylic acid ethyl ester 443984-41-6 443984-42-7 670274-03-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production

of TNF $\alpha$ )

IT 16217-18-8P 135829-04-8P, 1-Benzylloxycarbonylindoline-2-methanol  
 165807-04-5P 200184-60-7P, (S)-1-Benzylloxycarbonyl-4-methylidene proline Methyl Ester 290357-27-6P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-79-0P, 4-Ethoxycarbonyl-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-80-3P, 2-(4-Fluorophenyl)-4-hydroxymethyl-3-(pyridin-4-yl)-1H-pyrrole 321344-81-4P, 2-(4-Fluorophenyl)-4-formyl-3-(pyridin-4-yl)-1H-pyrrole 321344-83-6P, 4-(2-Cyanoethyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-84-7P, 4-[3-(tert-Butoxycarbonylamino)propyl]-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-86-9P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-1-(triisopropylsilyl)-1H-pyrrole 321344-87-0P, 4-Bromo-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321344-88-1P, [5-(4-Fluorophenyl)-4-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrol-3-yl] (pyridin-4-yl)methanol 321344-89-2P 321344-90-5P, 2-(4-Fluorophenyl)-4-(4-hydroxypiperidin-4-yl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321344-92-7P 321344-93-8P, 1-[1-(tert-Butoxycarbonyl)pyrrolidin-3-yl]-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-94-9P, 1-(1-(Diphenylmethyl)azetidin-3-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-95-0P, 1-(3-Benzyl oxypropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-96-1P, 3-(4-Fluorophenyl)-1-(3-hydroxypropyl)-2-(pyridin-4-yl)-1H-pyrrole 321344-97-2P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-[3-(4-toluenesulfonyloxy)propyl]-1H-pyrrole 321344-98-3P, 1-(3-Azidopropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole 321345-00-0P, 4-(2-Ethoxycarbonylethyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321345-01-1P, 2-(4-Fluorophenyl)-4-(3-hydroxypropyl)-3-(pyridin-4-yl)-1H-pyrrole 321345-02-2P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-[3-(4-toluenesulfonyloxy)propyl]-1H-pyrrole 321345-03-3P, 2-(4-Fluorophenyl)-4-(4-hydroxy-1-methylpiperidin-4-yl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-04-4P 321345-05-5P, 1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methylthiopyrimidin-4-yl)-1H-pyrrole 321345-06-6P, 1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methanesulfonyl)pyrimidin-4-yl)-1H-pyrrole 321345-07-7P, 1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methylaminopyrimidin-4-yl)-1H-pyrrole 321345-11-3P, 4-(3-Cyanopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321345-12-4P, 1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-fluoropyridin-4-yl)-1H-pyrrole 321345-13-5P, 1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methylaminopyridin-4-yl)-1H-pyrrole 321345-14-6P, 4-Bromo-2-(4-fluorophenyl)-3-(2-fluoropyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-15-7P 321345-16-8P, 4-(1-Allyloxycarbonyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-[2-((1S)-phenylethylamino)pyridin-4-yl]-1H-pyrrole 321345-17-9P, 4-Bromo-2-(4-fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-18-0P, 2-(4-Fluorophenyl)-3-(2-methylthiopyrimidin-4-yl)-1H-pyrrole 321345-19-1P, 2-(4-Fluorophenyl)-3-(2-(methanesulfonyl)pyrimidin-4-yl)-1H-pyrrole 321345-20-4P, 2-(4-Fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1H-pyrrole

321345-21-5P, 2-(4-Fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-22-6P, 3-[2-[N-(tert-Butoxycarbonyl)-N-methylamino]pyrimidin-4-yl]-2-(4-fluorophenyl)-1-triisopropylsilyl-1H-pyrrole 321345-23-7P, 4-Bromo-3-[2-(N-tert-butoxycarbonyl-N-methylamino)pyrimidin-4-yl]-2-(4-fluorophenyl)-1-triisopropylsilyl-1H-pyrrole 321345-24-8P, 4-Bromo-2-(4-fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1H-pyrrole 321345-25-9P, 4-Bromo-2-phenyl-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-26-0P, 4-Bromo-2-(3-chlorophenyl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-27-1P, 4-Bromo-2-(3-fluorophenyl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 321345-28-2P 321345-29-3P, 4-Bromo-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1-triisopropylsilyl-1H-pyrrole 335650-15-2P, (2S,4R)-1-Benzylloxycarbonyl-4-methoxy-2-hydroxymethylpyrrolidine 443685-77-6P 443912-06-9P, 3-[2-(4-Fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrol-4-yl]acrylonitrile 443912-07-0P, Ethyl 3-[2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrol-4-yl]acrylate 443912-08-1P, 2-(4-Fluorophenyl)-4-(3-hydroxy-1-propen-1-yl)-3-(pyridin-4-yl)-1H-pyrrole 443912-09-2P 443982-90-9P, (2R,8AS)-2-methoxy-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443982-93-2P 443982-96-5P, (2S,8AS)-2-chloro-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443982-99-8P, (8AS)-2,2-difluoro-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-03-7P, 6,7,8,9,9a,10-Hexahydropyrido[1,2-a]indol-8-one 443983-05-9P, (2R,8AS)-2-phenyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-11-7P 443983-16-2P 443983-20-8P 443983-24-2P 443983-28-6P, (2S,8AS)-2-methoxy-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-31-1P, (8AS)-2-methylidene-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-36-6P, (8AS)-2,2-dimethyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-42-4P, (8AS)-2-methyl-3,5,6,7,8,8a-hexahydroindolizin-7-one 443983-45-7P, (2S,8AS)-2-ethyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-47-9P, (2S,8AS)-2-butylthio-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-50-4P 443983-53-7P 443983-55-9P 443983-63-9P, (2S,8AS)-2-propyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-66-2P, (2R,8AS)-2-ethoxy-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-71-9P, (2S,8AS)-2-benzyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-74-2P 443983-77-5P, (2S,8AS)-2-phenoxy-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-85-5P 443983-86-6P, (2S,4R)-1-Benzylloxycarbonyl-2-cyanomethyl-4-methoxypyrrolidine 443983-88-8P, (2S,4R)-1-Benzylloxycarbonyl-2-(3-ethoxycarbonyl-2-oxopropyl)-4-methoxypyrrolidine 443983-89-9P, (2R,8AS)-2-Hydroxy-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443983-90-2P, 1-Benzylloxycarbonyl-2-cyanomethylindoline 443983-91-3P, 1-Benzylloxycarbonyl-2-(3-ethoxycarbonyl-2-oxopropyl)indoline 443983-93-5P, (S)-1-Benzylloxycarbonyl-2-hydroxymethyl-4-phenyl-3-pyrroline 443983-95-7P, (S)-1-Benzylloxycarbonyl-2-cyanomethyl-4-phenyl-3-pyrroline 443983-96-8P, (2S,4R)-1-Benzylloxycarbonyl-2-cyanomethyl-4-phenylpyrrolidine 443983-97-9P, (2S,4R)-1-Benzylloxycarbonyl-2-(3-(ethoxycarbonyl)-2-oxopropyl)-4-phenylpyrrolidine 443983-98-0P 443983-99-1P 443984-01-8P 443984-02-9P 443984-05-2P 443984-06-3P 443984-07-4P 443984-10-9P 443984-11-0P, (2S,8AS)-2-Methoxy-1,2,3,5,6,7,8,8a-octahydroindolizine-5,7-dione 443984-12-1P, (2S,8AS)-2-Methoxy-7-(1-pyrrolidinyl)-1,2,3,5,8,8a-hexahydroindolizin-5-one 443984-13-2P, (S)-1-Benzylloxycarbonyl-2-cyanomethyl-4-methylidenepyrrolidine 443984-14-3P, (S)-1-(tert-Butoxycarbonyl)-4-methylideneperidin-2-carboxylic acid ethyl ester 443984-16-5P, (2S,8AS)-2-methylthio-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443984-17-6P, (2S,4S)-1-Benzylloxycarbonyl-2-(tert-butyldimethylsilyloxy)methyl-4-acetylthiopyrrolidine 443984-19-8P 443984-20-1P, (2S,4S)-1-Benzylloxycarbonyl-2-hydroxymethyl-4-methylthiopyrrolidine 443984-21-2P, (2S,4S)-1-Benzylloxycarbonyl-2-cyanomethyl-4-methylthiopyrrolidine 443984-22-3P, (2S,4S)-4-(Methylthio)piperidin-2-carboxylic acid Hydrochloride 443984-23-4P, (2S,8AS)-2-methylsulfonyl-1,2,3,5,6,7,8,8a-octahydroindolizin-7-one 443984-28-9P, (S)-1-Benzylloxycarbonyl-4,4-

dimethyl-2-hydroxymethylpyrrolidine 443984-29-0P 443984-30-3P  
 443984-31-4P 443984-35-8P 443984-37-0P, (2S,4S)-1-Benzylloxycarbonyl-4-phenoxy piperidin-2-carboxylic acid benzyl ester 443984-40-5P,  
 (2S,4S)-4-Phenoxy piperidin-2-carboxylic acid Hydrochloride 465539-64-4P,  
 2-(4-Fluorophenyl)-4-(3-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-yl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole 471864-36-5P,  
 (2S,4R)-1-Benzylloxycarbonyl-4-methoxy-2-((methanesulfonyloxy)methyl)pyrrolidine 471864-42-3P, (2S,4R)-1-Benzylloxycarbonyl-2-(tert-butyldimethylsilyloxy)methyl-4-(p-toluenesulfonyloxy)pyrrolidine 476487-17-9P, (S)-4-Methylidene piperidin-2-carboxylic acid  
 Trifluoroacetate 651736-90-2P 670274-01-8P, 2-(3-Ethoxycarbonyl-2-oxononyl)indoline 670274-02-9P 670274-04-1P, (2S,4S)-4-Methoxy-1-(2-ethoxy-1,2-dioxoethyl)piperidin-2-carboxylic acid 670274-05-2P,  
 (2S,4R)-1-Benzylloxycarbonyl-2-hydroxymethyl-4-(p-toluenesulfonyloxy)pyrrolidine 670274-06-3P, (2S,4R)-1-Benzylloxycarbonyl-4-(p-toluenesulfonyloxy)pyrrolidin-2-carboxylic acid methyl ester 670274-07-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

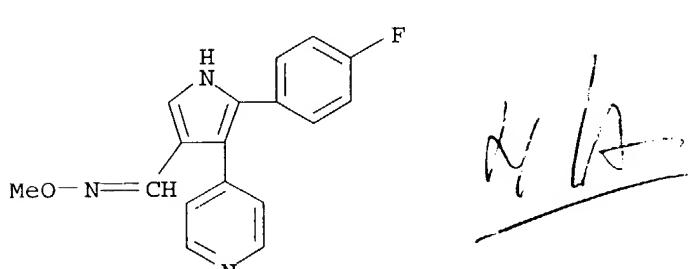
IT 321344-85-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrrole derivs. that inhibit production of TNF $\alpha$ )

RN 321344-85-8 HCPLUS

CN 1H-Pyrrole-3-carboxaldehyde, 5-(4-fluorophenyl)-4-(4-pyridinyl)-, O-methyloxime (9CI) (CA INDEX NAME)



L87 ANSWER 2 OF 4 HCPLUS COPYRIGHT 2004 ACS on STN

AN 2001:62383 HCPLUS

DN 134:115858

ED Entered STN: 26 Jan 2001

TI Preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines

IN Kimura, Tomio; Aoki, Kazumasa; Nakao, Akira; Ushiyama, Shigeru; Shimozato, Takaichi; Ohkawa, Nobuyuki

PA Sankyo Company Limited, Japan

SO Eur. Pat. Appl., 367 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D401-04

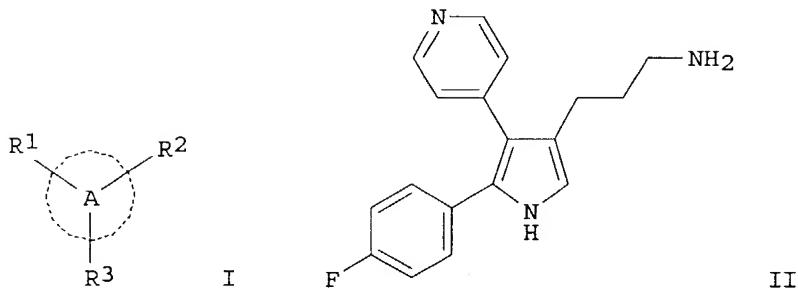
ICS C07D401-14; C07D453-02; C07D451-02; C07D471-04; C07D455-02; A61P011-06; A61P009-10; A61P017-06; A61P029-00; A61K031-4427; A61K031-4375

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1070711	A2	20010124	EP 2000-306196	20000720 <--
	EP 1070711	A3	20010131		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	NO 2000003734	A	20010122	NO 2000-3734	20000720 <--
	EP 1243589	A1	20020925	EP 2002-11912	20000720 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
	RU 2198170	C2	20030210	RU 2000-119431	20000720 <--
	AU 2000048755	A5	20010201	AU 2000-48755	20000721 <--
	ZA 2000003705	A	20010205	ZA 2000-3705	20000721 <--
	BR 2000004534	A	20010228	BR 2000-4534	20000721 <--
CN 1295069	A	20010516	CN 2000-131303	20000721 <--	
JP 2001247564	A2	20010911	JP 2000-220199	20000721 <--	
PRAI	JP 1999-205491	A	19990721 <--		
	JP 1999-369678	A	19991227 <--		
OS	EP 2000-306196	A3	20000720		
GI	MARPAT 134:115858				



AB The title compds. [I; A = pyrrole; R1 = (un)substituted aryl or heteroaryl; R2 = (un)substituted nitrogen-containing heteroaryl; R3 = XR4 (wherein X = a single bond, (un)substituted alkylene, alkenylene, alkynylene; R4 = substituted cycloalkyl, aryl, heterocyclyl, etc.); provided that said substituents R1 and R3 are bonded to the two atoms of said pyrrole ring which are adjacent to the atom of the pyrrole ring to which said substituent R2 is bonded] which have excellent inhibitory activity against the production of inflammatory cytokines such as TNF $\alpha$  (biol. data given) and IL-1 $\beta$ , and are useful in treating arthritis, were prepared and formulated. E.g., a multi-step synthesis of the pyrrole II was given.

ST pyrrole heteroaryl prep formulation inflammatory cytokine prodn inhibition; tumor necrosis factor alpha prodn inhibition pyrrole heteroaryl prep; TNF alpha prodn inhibition pyrrole heteroaryl prep; interleukin 1beta prodn inhibition pyrrole heteroaryl prep; antiarthritic pyrrole heteroaryl prep formulation

IT Antiarthritics  
(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

IT Interleukin 1 $\beta$   
Tumor necrosis factors  
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory

activity against the production of inflammatory cytokines)

IT 321343-74-2P 321343-78-6P 321343-82-2P 321343-83-3P 321343-86-6P  
 321343-87-7P 321343-98-0P 321344-06-3P 321344-09-6P 321344-17-6P  
 321344-19-8P 321344-24-5P 321344-26-7P 321344-28-9P 321344-33-6P  
 321344-37-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

IT 321343-75-3P 321343-76-4P 321343-77-5P 321343-79-7P 321343-80-0P  
 321343-81-1P 321343-84-4P 321343-88-8P 321343-89-9P 321343-90-2P  
 321343-91-3P 321343-92-4P 321343-93-5P 321343-94-6P 321343-95-7P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

IT 108-00-9, 2-Dimethylaminoethylamine 109-01-3, 1-Methylpiperazine  
 109-55-7, 3-Dimethylaminopropylamine 110-89-4, Piperidine, reactions  
 110-91-8, Morpholine, reactions 123-00-2, 4-Morpholinepropanamine  
 123-90-0, Thiomorpholine 532-24-1, 8-Methyl-8-azabicyclo[3.2.1]octan-3-one 700-16-3, Pentafluoropyridine 826-36-8, 2,2,6,6-Tetramethylpiperidin-4-one 867-13-0, Ethyl diethylphosphonoacetate  
 872-85-5, 4-Formylpyridine 1074-68-6, 4-Formyl-2-methylthiopyrimidine  
 1445-73-4, 1-Methylpiperidin-4-one 1465-76-5, 1-tert-Butylpiperidin-4-one 2407-99-0 2627-86-3, (S)-1-Phenylethylamine 2759-28-6,  
 1-Benzylpiperazine 3612-18-8, 1-Ethylpiperidin-4-one 3612-20-2,  
 1-Benzylpiperidin-4-one 3731-38-2, Quinuclidin-3-one 5355-68-0,  
 1-Isopropylpiperidin-4-one 5554-54-1, 1,2,2,6,6-Pentamethylpiperidin-4-one 6238-14-8, 3-Aminoquinuclidine 13669-32-4, 1,2-Dimethylpiperidin-4-one 16728-64-6, 3-Benzyl oxypropylamine 18942-89-7, 2-Nitroethyl acetate 21823-56-3, 2-Benzyl-1-methylpiperidin-4-one 23133-37-1,  
 1-Propylpiperidin-4-one 23581-42-2 24489-96-1, Ethyl 3-(4-pyridyl)acrylate 24654-55-5, 3-(4-Fluorophenyl)acrolein  
 28957-72-4, 8-Benzyl-8-azabicyclo[3.2.1]octan-3-one 36635-66-2  
 36768-62-4, 4-Amino-2,2,6,6-tetramethylpiperidine 39742-60-4,  
 1-Phenethylpiperidin-4-one 40114-49-6, 1-Benzylpiperidin-3-one  
 40432-52-8 50541-93-0, 4-Amino-1-benzylpiperidine 53369-71-4  
 71072-32-7, 1-Octylpiperidin-4-one 79538-29-7, 2,4,6-Trifluorobenzoyl chloride 96901-92-7, 3-Amino-8-benzyl-8-azabicyclo[3.2.1]octane  
 131747-69-8, 2-Fluoropyridin-4-carboxaldehyde 144222-22-0,  
 4-Aminomethyl-1-(tert-butoxycarbonyl)piperidine 162167-97-7  
 165806-95-1 184637-48-7, 3-Amino-1-(tert-butoxycarbonyl)piperidine  
 186550-13-0, 3-Amino-1-(tert-butoxycarbonyl)pyrrolidine 190906-83-3,  
 2-Methyl-1-propylpiperidin-4-one 203661-73-8, 1-Benzyl-2-methylpiperidin-4-one 247570-24-7 263389-45-3 306296-67-3, 1-

Allyloxycarbonylpiperidin-4-one 321345-30-6, 4-Amino-1-benzyl-2-methylpiperidine 321345-31-7, Ethyl 3-(2-fluoropyridin-4-yl)acrylate 321345-32-8, 1-Ethyl-2-methylpiperidin-4-one 321345-33-9, 2-Allyl-1-methylpiperidin-4-one 321345-34-0, Ethyl 3-(2-methylthiopyrimidin-4-yl)acrylate 321345-35-1 321345-36-2 321345-37-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

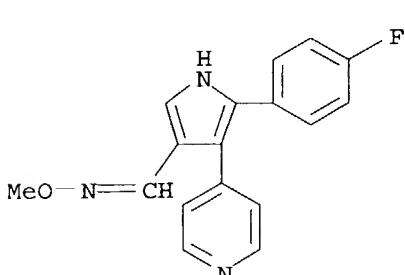
(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

IT **321344-85-8P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

RN 321344-85-8 HCAPLUS

CN 1H-Pyrrole-3-carboxaldehyde, 5-(4-fluorophenyl)-4-(4-pyridinyl)-, O-methyloxime (9CI) (CA INDEX NAME)



L87 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:473973 HCAPLUS

DN 129:108993

ED Entered STN: 30 Jul 1998

TI Preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression.

IN Kawai, Akiyoshi; Kawai, Makoto

PA Pfizer Inc., USA

SO Eur. Pat. Appl., 53 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D409-04

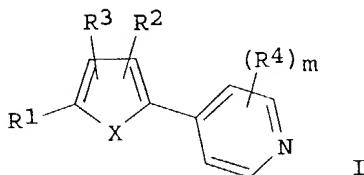
ICS C07D405-04; C07D493-04; C07D409-14; C07D495-04; A61K031-44

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 853083	A1	19980715	EP 1997-310375	19971219 <--
PI EP 853083	B1	20010912		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PT 853083	T	20011228	PT 1997-97310375	19970106 <--
AT 205494	E	20010915	AT 1997-310375	19971219 <--
ES 2161418	T3	20011201	ES 1997-310375	19971219 <--
JP 10195070	A2	19980728	JP 1997-366682	19971226 <--
JP 3384962	B2	20030310		
CA 2226039	AA	19980706	CA 1997-2226039	19971231 <--
BR 9800228	A	19990908	BR 1998-228	19980106 <--
US 6048880	A	20000411	US 1998-3108	19980106 <--
US 2002022729	A1	20020221	US 2001-918153	20010730 <--
US 6696470	B2	20040224		
GR 3037073	T3	20020131	GR 2001-401945	20011030 <--
PRAI WO 1997-IB2	W	19970106	<--	
US 1998-3108	A1	19980106	<--	
US 1999-317570	B1	19990524	<--	
OS MARPAT 129:108993				
GI				



AB Title compds. [I; R<sub>1</sub>, R<sub>2</sub> = H, halo, (substituted) (cyclo)alkyl, hydroxy(cyclo)alkyl, alkoxy, alkenyl, alkynyl, (substituted) heterocyclyl, (hetero)aryl, acyl, cyano, NO<sub>2</sub>, aminocarbonyl, etc.; R<sub>3</sub> = (substituted) (cyclo)alkyl, (cyclo)alkylcarbonyl, cyano, formyl, alkenylcarbonyl, alkynylcarbonyl, arylcarbonyl, etc.; R<sub>4</sub> = H, halo, alkyl, hydroxyalkyl, alkylcarbonyl, etc.; 2 of R<sub>1</sub>-R<sub>3</sub> = atoms to form (substituted) rings; X = O, S, SO, SO<sub>2</sub>; m = 0-4; and N-oxides thereof], were prepared. Thus, 3-acetyl-2,4-dimethylfuran was refluxed with NBS and AIBN in benzene for 1 h to give 88% 3-acetyl-5-bromo-2,4-dimethylfuran. The latter in dimethoxyethane was refluxed with aqueous NaHCO<sub>3</sub> and (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> followed by addition of 4-pyridineboronic acid and (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> and further reflux to give 31% 3-acetyl-2,4-dimethyl-5-(4-pyridyl)furan. Selected I inhibited TNF $\alpha$  biosynthesis with IC<sub>50</sub> = 100 nM to 10  $\mu$ M.

ST pyridylfuran pyridylthiophene prepn TNF biosynthesis inhibitor; cell adhesion mol expression inhibitor pyridylfuran; drug pyridylfuran pyridylthiophene prepn

IT AIDS (disease)

(-related complex, drugs for; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Intestine, disease

(Crohn's, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Antiarteriosclerotics

(antiatherosclerotics; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Tumor necrosis factors

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(biosynthesis inhibitors; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Malaria  
 Malaria  
     (cerebral, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Intestine, disease  
     (inflammatory, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Cell adhesion  
     (inhibitors; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Reperfusion  
     (injury, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Brain, disease  
 Brain, disease  
     (malaria, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Respiratory distress syndrome  
     (newborn, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Allergy inhibitors  
     **Anti-AIDS agents**  
     Anti-inflammatory agents  
     Antiarthritis  
     Antiasthmatics  
     Anticoagulants  
     Antidiabetic agents  
     Antimalarials  
     Antibesity agents  
     Antipyretics  
     Antitumor agents  
         **Antiviral agents**  
     Cardiovascular agents  
         (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Bone  
     (resorption, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Shock (circulatory collapse)  
     (septic, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Shock (circulatory collapse)  
     (toxic shock syndrome, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Cachexia  
 Keloid  
 Psoriasis  
 Sepsis  
 Silicosis  
 Skin, disease  
 Transplant rejection  
     (treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT Intestine, disease  
     (ulcerative colitis, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT 210096-98-3P 210097-13-5P 210097-28-2P 210097-33-9P 210097-47-5P  
 210097-55-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT 207307-41-3P 210096-99-4P 210097-00-0P 210097-02-2P 210097-03-3P  
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**210097-62-4P** 210097-63-5P 210097-64-6P 210097-65-7P  
 210097-66-8P 210097-67-9P 210097-68-0P 210097-69-1P 210097-70-4P  
 210097-71-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT 74-89-5, Methylamine, reactions 75-16-1, Methylmagnesium bromide  
 98-80-6, Benzeneboronic acid 103-67-3, N-Methylbenzylamine 105-53-3,  
 Diethyl malonate 108-30-5, reactions 108-95-2, Phenol, reactions  
 109-01-3, N-Methylpiperazine 110-89-4, Piperidine, reactions 110-91-8,  
 Morpholine, reactions 116-09-6, Hydroxyacetone 124-40-3,  
 Dimethylamine, reactions 367-12-4, 2-Fluorophenol 371-41-5,  
 4-Fluorophenol 504-02-9, 1,3-Cyclohexanedione 562-46-9,  
 4,4-Dimethyl-1,3-Cyclohexanedione 593-56-6, Methoxylamine hydrochloride  
 616-44-4, 3-Methylthiophene 638-00-6, 2,4-Dimethylthiophene 917-54-4,  
 Methylolithium 1194-18-9, 1,3-Cycloheptanenedione 1641-09-4,  
 3-Cyanothiophene 1679-18-1, 4-Chlorobenzeneboronic acid 1692-15-5,  
 4-Pyridineboronic acid 1692-25-7, 3-Pyridineboronic acid 1765-93-1,  
 4-Fluorobenzeneboronic acid 1993-03-9 2713-31-7, 2,5-Difluorophenol  
 3172-52-9, 2,5-Dichlorothiophene 4414-45-3 5077-67-8,  
 1-Hydroxy-2-butanone 5720-07-0, 4-Methoxybenzeneboronic acid  
 6165-69-1, 3-Thiopheneboronic acid 25074-25-3 30318-99-1,  
 3-Bromo-4-methylthiophene 32933-07-6, 3-Acetyl-2,4-dimethylfuran  
 33177-29-6 36157-40-1, 3-Acetyl-2,5-dichlorothiophene 39177-23-6,  
 3-(4-Fluorophenoxy)phenol 41903-50-8, Hydroxyacetophenone 57248-14-3,  
 2,5-Dichloro-3-thiophenecarbonyl chloride 69213-94-1 69213-95-2  
 85006-25-3 98546-51-1 128796-39-4, 4-Trifluoromethylbenzeneboronic  
 acid 145129-54-0 207307-53-7 210098-25-2 210098-26-3 210098-27-4  
 210098-28-5 210098-30-9 210098-31-0 210098-32-1 210098-33-2  
 210098-34-3 210098-36-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

IT 6906-61-2P 7687-77-6P 7687-78-7P 7687-79-8P 7690-96-2P  
 17249-90-0P, 2,5-Dichloro-3-methylthiophene 18792-01-3P 19945-43-8P  
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 39712-65-7P 39712-66-8P 63826-64-2P 63826-68-6P 66577-03-5P  
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 210098-24-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

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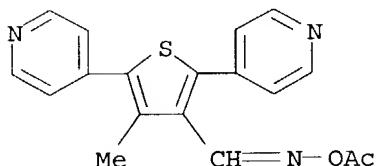
- (1) Bacon, E; J HETEROCYCL CHEM 1991, V28(8), P1953 HCPLUS
- (2) Gilat, S; J CHEM SOC, CHEM COMMUN 1993, 18, P1439 HCPLUS
- (3) Katritzky, A; ENERGY FUELS 1990, V4(5), P572 HCPLUS
- (4) Oda, K; J CHEM SOC, CHEM COMMUN 1994, 12, P1477 HCPLUS
- (5) Pfizer Pharma; WO 9802430 A HCPLUS
- (6) Ribereau, P; C R HEBD SEANCES ACAD SCI, SER C 1975, V280(5), P293 HCPLUS
- (7) Zhang, Y; J HETEROCYCL CHEM 1993, V30(5), P1293 HCPLUS

IT 210097-56-6P 210097-62-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF $\alpha$  biosynthesis and CAMs expression)

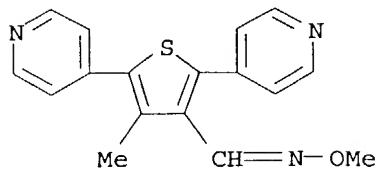
RN 210097-56-6 HCPLUS

CN 3-Thiophenecarboxaldehyde, 4-methyl-2,5-di-4-pyridinyl-, O-acetyloxime (9CI) (CA INDEX NAME)



RN 210097-62-4 HCPLUS

CN 3-Thiophenecarboxaldehyde, 4-methyl-2,5-di-4-pyridinyl-, O-methyloxime, dihydrochloride (9CI) (CA INDEX NAME)



*[Handwritten signature]*

●2 HCl

L87 ANSWER 4 OF 4 HCPLUS COPYRIGHT 2004 ACS on STN

AN 1993:51800 HCPLUS

DN 118:51800

ED Entered STN: 16 Feb 1993

TI Oxidation of carbovir, a carbocyclic nucleoside, by rat liver cytosolic enzymes. Enantioselectivity and enantiomeric inhibition

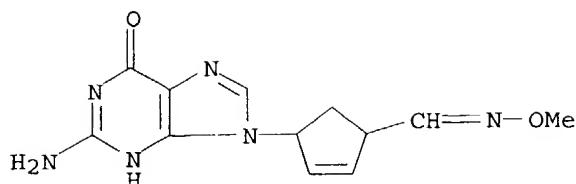
AU Patanella, James E.; Walsh, John S.

CS Res. Inst., Glaxo, Inc., Research Triangle Park, NC, USA  
 SO Drug Metabolism and Disposition (1992), 20(6), 912-19  
 CODEN: DMDSAI; ISSN: 0090-9556

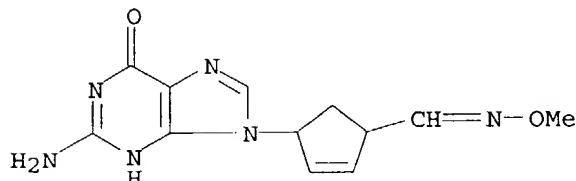
DT Journal  
 LA English  
 CC 1-2 (Pharmacology)

AB Previous metabolism studies of (-)-cis-carbovir (1'R-cis-2-amino-1,9-dihydro-9-[4'S-hydroxymethyl-2-cyclopenten-1-yl]-6H-purin-6-one), an antiviral agent, have shown that the major route of metabolism of carbovir in the rat is oxidation of the methylene hydroxyl group of the cyclopentadiene ring to form the corresponding 4'-carboxylic acid metabolite. We have determined that rat hepatic alc. dehydrogenase and aldehyde dehydrogenase are responsible for this biotransformation through sequential oxidation of the alc. through the aldehyde to the carboxylic acid. The results of incubations of racemic ( $\pm$ )-cis-carbovir with rat liver cytosol showed that this oxidation occurs enantioselectively favoring the (+)-enantiomer by a factor of 6- to 7-fold. We have proven that alc. dehydrogenase contributes to the enantioselectivity of the overall oxidation process, but were unable to determine whether or not any contribution is made by aldehyde dehydrogenase. Parallel incubations conducted with the sep. enantiomers revealed that the concentration required to achieve a half-maximal rate for the oxidation of the (+)-enantiomer (0.27 mM) was one-fifth that required for the (-)-enantiomer (1.36 mM). Results from enantiomeric inhibition studies showed that (+)-carbovir inhibited the oxidation of (-)-carbovir. In contrast, (-)-carbovir did not inhibit the oxidation of (+)-carbovir.

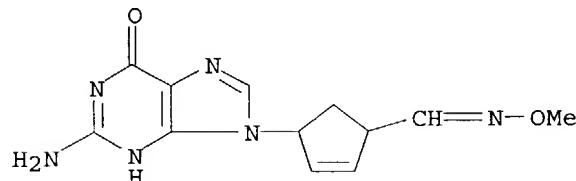
ST carbovir oxidn liver  
 IT Liver, metabolism  
     (carbovir metabolism in, enantioselectivity and enantiomeric inhibition in)  
 IT 9028-86-8, Aldehyde dehydrogenase  
     RL: BIOL (Biological study)  
     (carbovir aldehyde intermediate oxidation by, enantioselectivity of)  
 IT 9031-72-5, Alcohol dehydrogenase  
     RL: RCT (Reactant); RACT (Reactant or reagent)  
     (carbovir oxidation by, enantioselectivity of)  
 IT 131956-47-3 132012-22-7 145414-80-8 145414-81-9  
     RL: FORM (Formation, nonpreparative)  
     (formation of, as carbovir conjugative metabolite, enantioselectivity and enantiomeric inhibition in)  
 IT 145414-78-4  
     RL: FORM (Formation, nonpreparative)  
     (formation of, as carbovir oxidative metabolite, enantioselectivity and enantiomeric inhibition in)  
 IT 118353-05-2  
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
     (metabolism of, in liver, enantioselectivity and enantiomeric inhibition in)  
 IT 120443-30-3, (-)-Carbovir 124915-24-8, (+)-Carbovir  
     RL: RCT (Reactant); RACT (Reactant or reagent)  
     (oxidation of, by alc. dehydrogenase, enantioselectivity in)  
 IT 145356-37-2P 145414-79-5P  
     RL: SPN (Synthetic preparation); PREP (Preparation)  
     (preparation of, as carbovir aldehyde intermediate trap)  
 IT 145414-80-8 145414-81-9  
     RL: FORM (Formation, nonpreparative)  
     (formation of, as carbovir conjugative metabolite, enantioselectivity and enantiomeric inhibition in)  
 RN 145414-80-8 HCAPLUS  
 CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(O-methyloxime), [1R-[1 $\alpha$ (E), 4 $\alpha$ ]]- (9CI) (CA INDEX NAME)



RN 145414-81-9 HCPLUS  
 CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(O-methyloxime), [1R-[1 $\alpha$ (Z),4 $\alpha$ ]]- (9CI) (CA INDEX NAME)

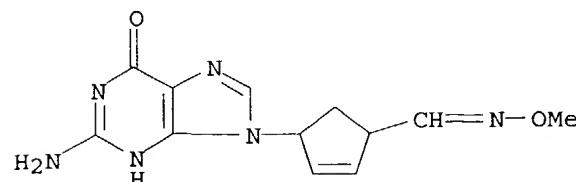


IT 145356-37-2P 145414-79-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as carbovir aldehyde intermediate trap)  
 RN 145356-37-2 HCPLUS  
 CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(O-methyloxime), [1S-[1 $\alpha$ (Z),4 $\alpha$ ]]- (9CI) (CA INDEX NAME)



*[Handwritten signature]*

RN 145414-79-5 HCPLUS  
 CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(O-methyloxime), [1S-[1 $\alpha$ (E),4 $\alpha$ ]]- (9CI) (CA INDEX NAME)



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